

Title of Invention: Aromatic Oxyphenyl and Aromatic Sulfanyphenyl Derivatives
Inventors (please provide full names): Graciek Smith, Gille Mikkelsen,
Kim Andersen, Daniel Grue & Torgun Eskildsen
Earliest Priority Date: 4/30/03

Search Topic:

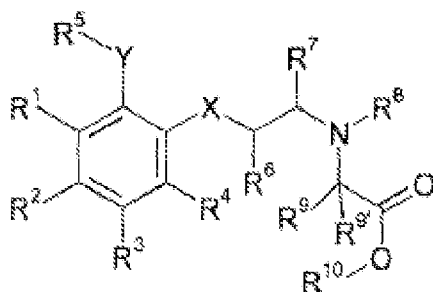
Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Please search claim 1. Thank you!

1. (Pre)

1. (Pre)



wherein

X is O, S or CR¹¹R¹², wherein R¹¹ and R¹² are each independently H or C₁₋₆ alkyl;

Y is 0 or S;

R¹, R², R³ and R⁴ are each independently hydrogen; halogen; cyano; nitro; C₁₋₆-alk(en/yn)yl; C₁₋₆-alk(en/yn)yloxy; C₁₋₆-alk(en/yn)ylsulfanyl; hydroxy; hydroxy-C₁₋₆-alk(en/yn)yl; halo-C₁₋₆-alk(en/yn)yl; halo-C₁₋₆-alk(en/yn)yloxy; C₃₋₈-cycloalk(en)yl; C₃₋₈-cycloalk(en)yl-C₁₋₆-alk(en/yn)yl; acyl; C₁₋₆-alk(en/yn)yloxycarbonyl; C₁₋₆-alk(en/yn)ylsulfonyl; aryl optionally substituted with a halogen, cyano, nitro, C₁₋₆-alk(en/yn)yl, C₁₋₆-alk(en/yn)yloxy, C₃₋₆-alk(en/yn)ylsulfanyl, hydroxy, hydroxy-C₁₋₆-alk(en/yn)yl, halo-C₁₋₆-alk(en/yn)yl, halo-C₁₋₆-alk(en/yn)yloxy, C₃₋₈-cycloalk(en)yl, C₃₋₈-cycloalk(en)yl-C₁₋₆-alk(en/yn)yl, acyl, C₁₋₆-alk(en/yn)yloxycarbonyl or C₁₋₆-alk(en/yn)ylsulfonyl; monocyclic heteroaryl optionally substituted with a halogen, cyano, nitro, C₁₋₆-alk(en/yn)yl, C₁₋₆-alk(en/yn)yloxy, C₃₋₆-alk(en/yn)ylsulfanyl, hydroxy, hydroxy-C₁₋₆-alk(en/yn)yl, halo-C₁₋₆-alk(en/yn)yl, halo-C₃₋₆-alk(en/yn)yloxy, C₃₋₈-cycloalk(en)yl, C₃₋₈-cycloalk(en)yl-C₁₋₆-alk(en/yn)yl, acyl, C₁₋₆-

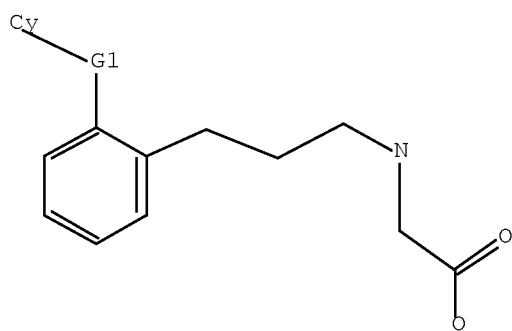
***** INVENTOR RESULTS *****

=> d his 123

(FILE 'HCAPLUS' ENTERED AT 13:11:11 ON 26 MAR 2009)
L23 2 S ((L18-L22) AND L15) OR (L15 AND L16)

=> d que 123

L5 STR

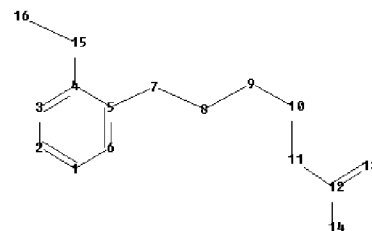
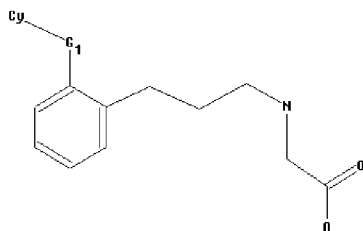


G1 O,S

Structure attributes must be viewed using STN Express query preparation:

Uploading L3.str

10/551737



```

chain nodes :
7 12 13 14 15 16
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
8 9 10 11
chain bonds :
4-15 5-7 7-8 11-12 12-13 12-14 15-16
ring/chain bonds :
8-9 9-10 10-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
4-15 8-9 9-10 10-11 12-13 12-14 15-16
exact bonds :
5-7 7-8 11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

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G1:O,S

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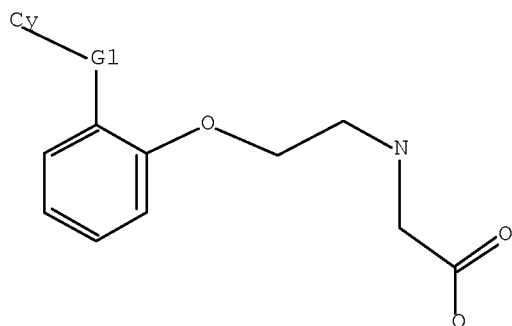
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1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom
Generic attributes :
16:
Type of Ring System : Monocyclic

```

L9

STR

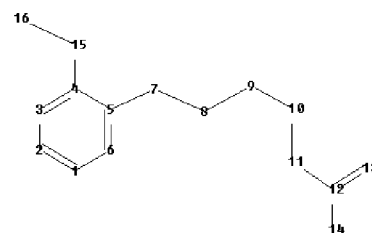
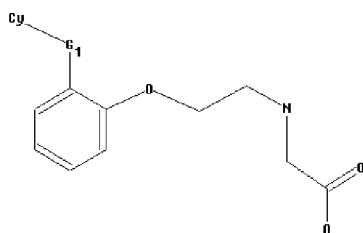
10/551737



G1 O,S

Structure attributes must be viewed using STN Express query preparation:

Uploading L5.str



```
chain nodes :
7 12 13 14 15 16
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
8 9 10 11
chain bonds :
4-15 5-7 7-8 11-12 12-13 12-14 15-16
ring/chain bonds :
8-9 9-10 10-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
4-15 5-7 7-8 8-9 9-10 10-11 12-13 12-14 15-16
exact bonds :
11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :
```

G1:O,S

10/551737

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom

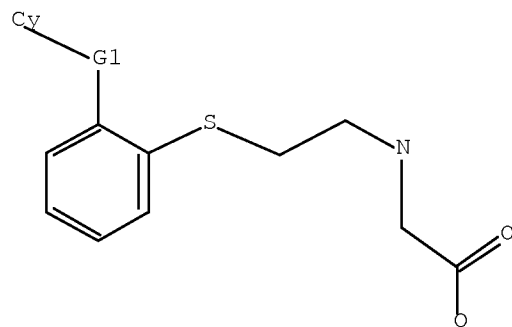
Generic attributes :

16:

Type of Ring System : Monocyclic

L11

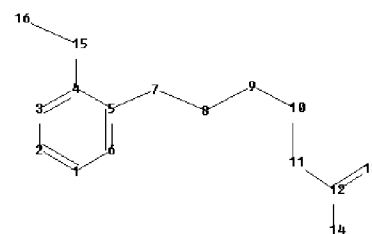
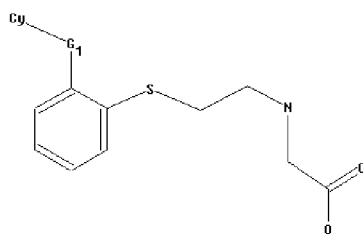
STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation:

Uploading L6.str



chain nodes :

7 12 13 14 15 16

ring nodes :

1 2 3 4 5 6

ring/chain nodes :

8 9 10 11

chain bonds :

4-15 5-7 7-8 11-12 12-13 12-14 15-16

ring/chain bonds :

8-9 9-10 10-11
 ring bonds :
 1-2 1-6 2-3 3-4 4-5 5-6
 exact/norm bonds :
 4-15 5-7 7-8 8-9 9-10 10-11 12-13 12-14 15-16
 exact bonds :
 11-12
 normalized bonds :
 1-2 1-6 2-3 3-4 4-5 5-6
 isolated ring systems :
 containing 1 :

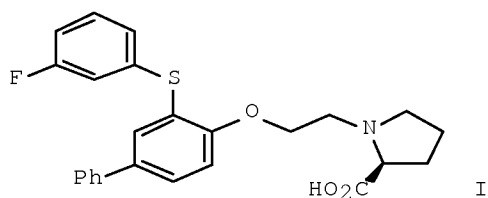
G1:O,S

Match level :
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom
 Generic attributes :
 16:
 Type of Ring System : Monocyclic

L14 171 SEA FILE=REGISTRY SSS FUL L5 OR L9 OR L11
 L15 11 SEA FILE=HCAPLUS ABB=ON PLU=ON L14
 L16 1 SEA FILE=HCAPLUS ABB=ON PLU=ON US20060235003/PN
 L18 6 SEA FILE=HCAPLUS ABB=ON PLU=ON SMITH GARRICK/AU
 L19 17 SEA FILE=HCAPLUS ABB=ON PLU=ON MIKKELSEN G?/AU
 L20 71 SEA FILE=HCAPLUS ABB=ON PLU=ON ANDERSEN KIM/AU
 L21 203 SEA FILE=HCAPLUS ABB=ON PLU=ON GREVE D?/AU
 L22 19 SEA FILE=HCAPLUS ABB=ON PLU=ON ESKILDSSEN J?/AU
 L23 2 SEA FILE=HCAPLUS ABB=ON PLU=ON ((L18 OR L19 OR L20 OR L21
 OR L22)) AND L15) OR (L15 AND L16)

=> d 123 1-2 ibib abs hitstr

L23 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2006:625349 HCAPLUS Full-text
 DOCUMENT NUMBER: 145:224321
 TITLE: The synthesis and SAR of
 2-arylsulfanyphenyl-1-oxyalkylamino acids as GlyT-1
 inhibitors
 AUTHOR(S): Smith, Garrick; Mikkelsen, Gitte;
 Eskildsen, Jorgen; Bundgaard, Christoffer
 CORPORATE SOURCE: Medicinal Chemistry Research, H. Lundbeck A/S, Valby,
 DK 2500, Den.
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2006),
 16(15), 3981-3984
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 145:224321
 GI



AB Elevation of glycine levels by inhibition of the glycine transporter-1 (GlyT-1) and activation of the NMDA receptor is a potential strategy for the treatment of schizophrenia. A novel series of 2-arylsulfanylphenyl-1-oxyalkyl amino acids have been identified. The most prominent member of this series (I) is a potent GlyT-1 inhibitor ($IC_{50} = 59 \text{ nM}$). In vitro and in vivo assessment of CNS exposure indicates this compound is a likely substrate for active efflux transporters.

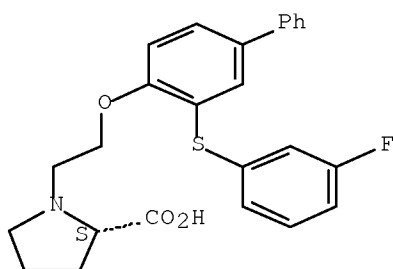
IT 791644-20-7P 791644-21-8P

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and SAR of arylsulfanylphenyloxyalkylamino acids as GlyT-1 inhibitors)

RN 791644-20-7 HCAPLUS

CN L-Proline, 1-[2-[[3-[(3-fluorophenyl)thio][1,1'-biphenyl]-4-yl]oxy]ethyl]- (CA INDEX NAME)

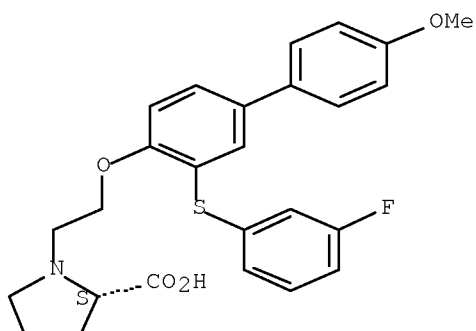
Absolute stereochemistry.



RN 791644-21-8 HCAPLUS

CN L-Proline, 1-[2-[[3-[(3-fluorophenyl)thio]-4'-methoxy[1,1'-biphenyl]-4-yl]oxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



IT 791642-87-0P 791643-06-6P 791643-10-2P
 791643-25-9P 791643-27-1P 791643-31-7P
 791643-68-0P 791644-17-2P 791644-18-3P
 794510-03-5P 905815-53-4P 905815-54-5P
 905815-55-6P 905815-56-7P 905815-57-8P
 905815-58-9P 905815-59-0P 905815-60-3P
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 905815-64-7P 905815-65-8P 905815-66-9P
 905815-67-0P

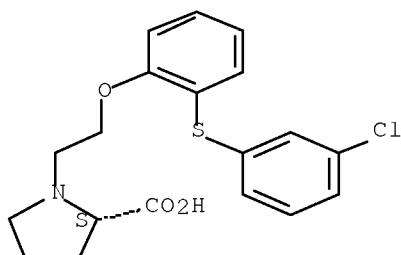
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(synthesis and SAR of arylsulfanylphenoxyalkylamino acids as GlyT-1
 inhibitors)

RN 791642-87-0 HCAPLUS

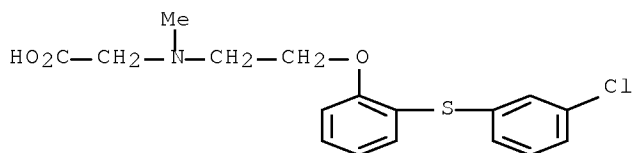
CN L-Proline, 1-[2-[2-[(3-chlorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



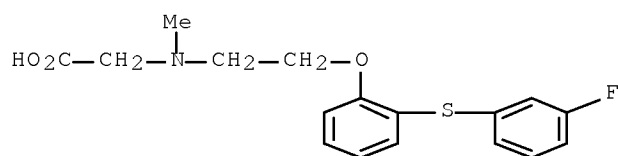
RN 791643-06-6 HCAPLUS

CN Glycine, N-[2-[2-[(3-chlorophenyl)thio]phenoxy]ethyl]-N-methyl- (CA INDEX NAME)



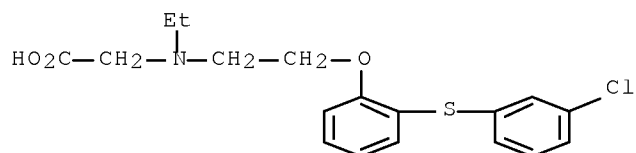
RN 791643-10-2 HCAPLUS

CN Glycine, N-[2-[2-[(3-fluorophenyl)thio]phenoxy]ethyl]-N-methyl- (CA INDEX NAME)



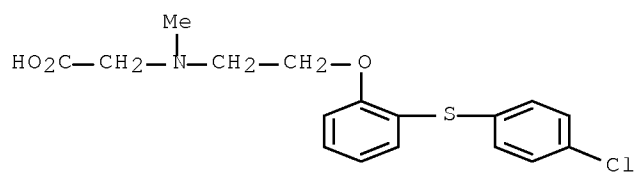
RN 791643-25-9 HCAPLUS

CN Glycine, N-[2-[2-[(3-chlorophenyl)thio]phenoxy]ethyl]-N-ethyl- (CA INDEX NAME)



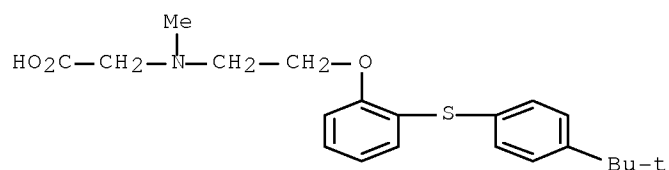
RN 791643-27-1 HCAPLUS

CN Glycine, N-[2-[2-[(4-chlorophenyl)thio]phenoxy]ethyl]-N-methyl- (CA INDEX NAME)



RN 791643-31-7 HCAPLUS

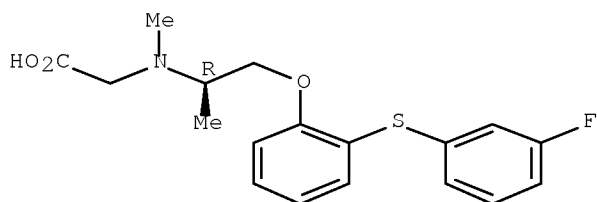
CN Glycine, N-[2-[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]ethyl]-N-methyl- (CA INDEX NAME)



RN 791643-68-0 HCAPLUS

CN Glycine, N-[(1R)-2-[2-[(3-fluorophenyl)thio]phenoxy]-1-methylethyl]-N-methyl- (CA INDEX NAME)

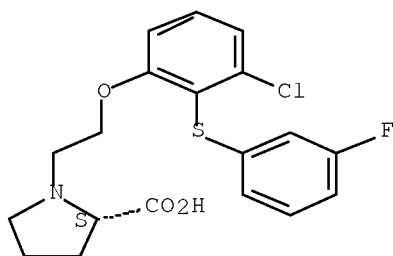
Absolute stereochemistry.



RN 791644-17-2 HCAPLUS

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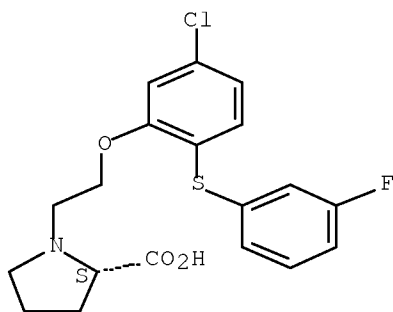
Absolute stereochemistry.



RN 791644-18-3 HCAPLUS

CN L-Proline, 1-[2-[5-chloro-2-[(3-fluorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.

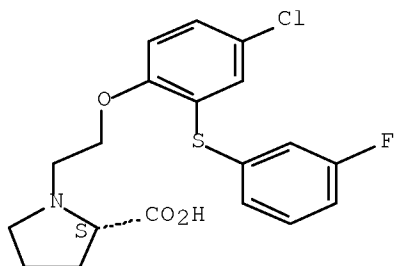


10/551737

RN 794510-03-5 HCAPLUS

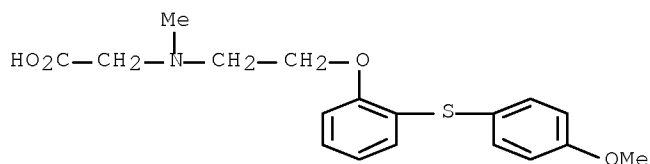
CN L-Proline, 1-[2-[4-chloro-2-[(3-fluorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



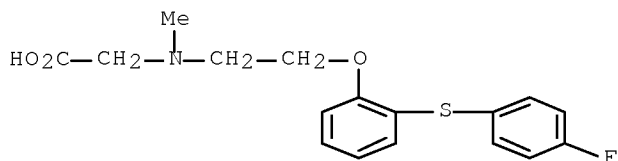
RN 905815-53-4 HCAPLUS

CN Glycine, N-[2-[2-[(4-methoxyphenyl)thio]phenoxy]ethyl]-N-methyl- (CA INDEX NAME)



RN 905815-54-5 HCAPLUS

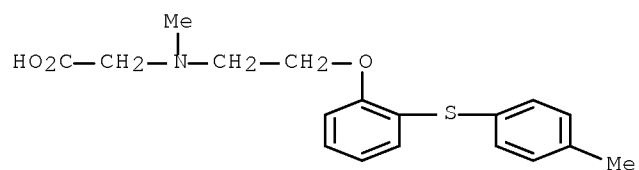
CN Glycine, N-[2-[2-[(4-fluorophenyl)thio]phenoxy]ethyl]-N-methyl- (CA INDEX NAME)



RN 905815-55-6 HCAPLUS

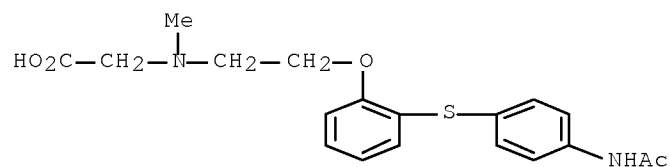
CN Glycine, N-methyl-N-[2-[2-[(4-methylphenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

10/551737



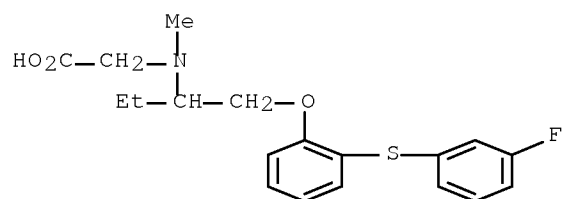
RN 905815-56-7 HCAPLUS

CN Glycine, N-[2-[2-[[4-(acetylamino)phenyl]thio]phenoxy]ethyl]-N-methyl-
(CA INDEX NAME)



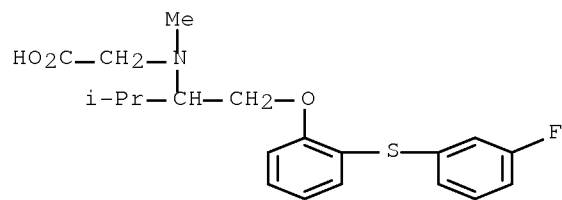
RN 905815-57-8 HCAPLUS

CN Glycine, N-[1-[[2-[(3-fluorophenyl)thio]phenoxy]methyl]propyl]-N-methyl-
(CA INDEX NAME)



RN 905815-58-9 HCAPLUS

CN Glycine, N-[1-[[2-[(3-fluorophenyl)thio]phenoxy]methyl]-2-methylpropyl]-N-methyl-
(CA INDEX NAME)

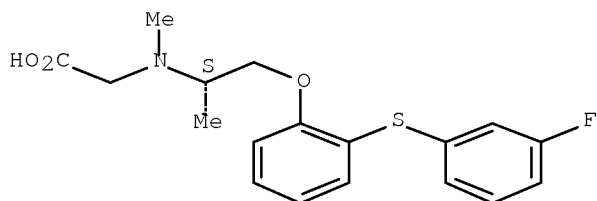


RN 905815-59-0 HCAPLUS

10/551737

CN Glycine, N-[(1S)-2-[2-[(3-fluorophenyl)thio]phenoxy]-1-methylethyl]-N-methyl- (CA INDEX NAME)

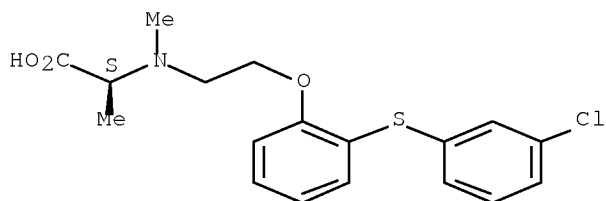
Absolute stereochemistry.



RN 905815-60-3 HCAPLUS

CN L-Alanine, N-[2-[2-[(3-chlorophenyl)thio]phenoxy]ethyl]-N-methyl- (CA INDEX NAME)

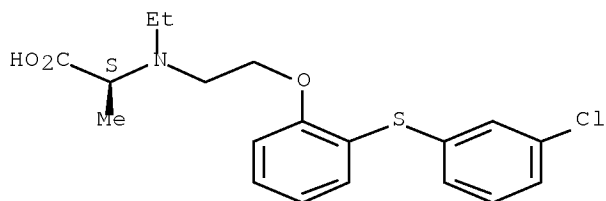
Absolute stereochemistry.



RN 905815-61-4 HCAPLUS

CN L-Alanine, N-[2-[2-[(3-chlorophenyl)thio]phenoxy]ethyl]-N-ethyl- (CA INDEX NAME)

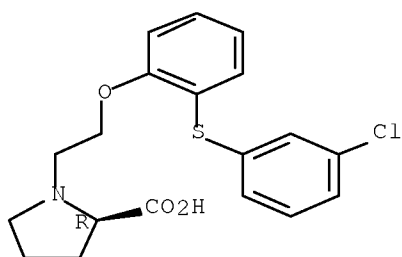
Absolute stereochemistry.



RN 905815-62-5 HCAPLUS

CN D-Proline, 1-[2-[2-[(3-chlorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

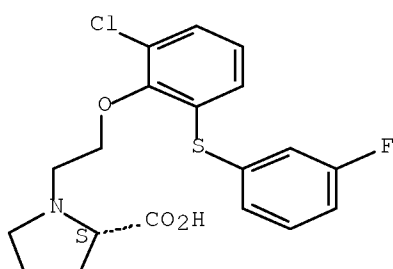
Absolute stereochemistry.



RN 905815-63-6 HCAPLUS

CN L-Proline, 1-[2-[2-chloro-6-[(3-fluorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

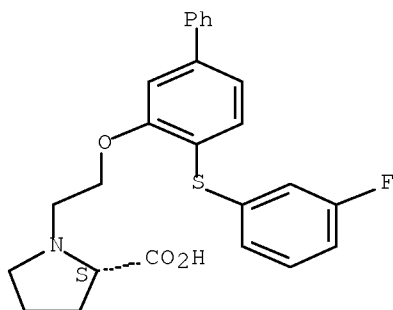
Absolute stereochemistry.



RN 905815-64-7 HCAPLUS

CN L-Proline, 1-[2-[4-[(3-fluorophenyl)thio][1,1'-biphenyl]-3-yl]oxy]ethyl]- (CA INDEX NAME)

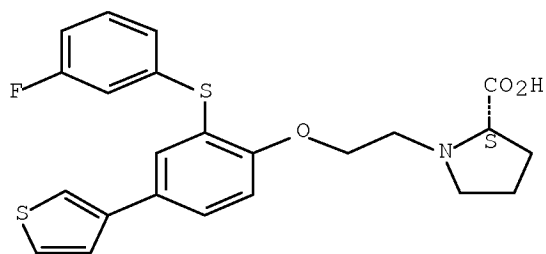
Absolute stereochemistry.



RN 905815-65-8 HCAPLUS

CN L-Proline, 1-[2-[2-[(3-fluorophenyl)thio]-4-(3-thienyl)phenoxy]ethyl]- (CA INDEX NAME)

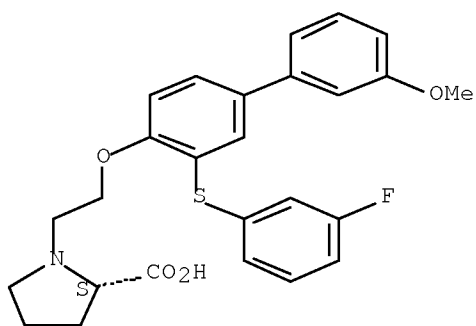
Absolute stereochemistry.



RN 905815-66-9 HCAPLUS

CN L-Proline, 1-[2-[[3-[(3-fluorophenyl)thio]-3'-methoxy[1,1'-biphenyl]-4-yl]oxy]ethyl]- (CA INDEX NAME)

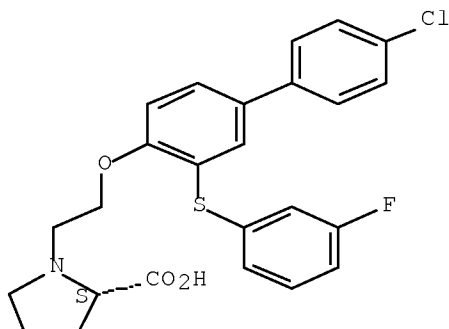
Absolute stereochemistry.



RN 905815-67-0 HCAPLUS

CN L-Proline, 1-[2-[[4'-chloro-3-[(3-fluorophenyl)thio][1,1'-biphenyl]-4-yl]oxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



IT 791642-79-0P 791644-01-4P 905816-02-6P
 905816-03-7P 905816-06-0P 905816-07-1P
 905816-08-2P 905816-09-3P

10/551737

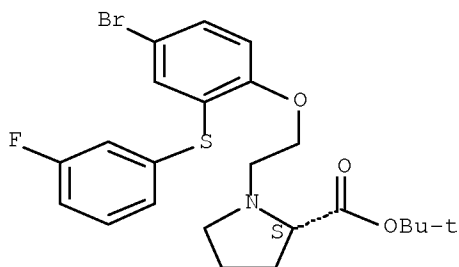
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and SAR of arylsulfanylphenyloxyalkylamino acids as GlyT-1 inhibitors)

RN 791642-79-0 HCAPLUS

CN L-Proline, 1-[2-[4-bromo-2-[(3-fluorophenyl)thio]phenoxy]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

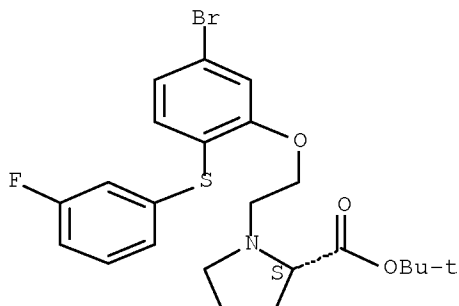
Absolute stereochemistry.



RN 791644-01-4 HCAPLUS

CN L-Proline, 1-[2-[5-bromo-2-[(3-fluorophenyl)thio]phenoxy]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

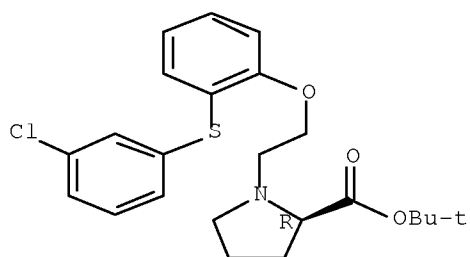
Absolute stereochemistry.



RN 905816-02-6 HCAPLUS

CN D-Proline, 1-[2-[2-[(3-chlorophenyl)thio]phenoxy]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

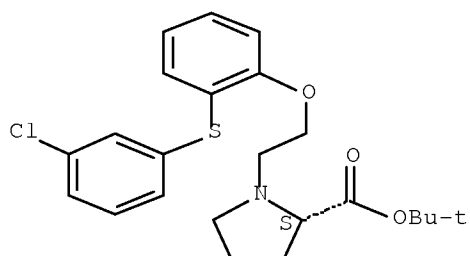
Absolute stereochemistry.



RN 905816-03-7 HCAPLUS

CN L-Proline, 1-[2-[2-[(3-chlorophenyl)thio]phenoxy]ethyl]-,
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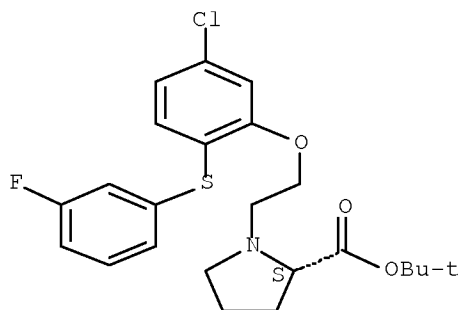
Absolute stereochemistry.



RN 905816-06-0 HCAPLUS

CN L-Proline, 1-[2-[2-[(3-fluorophenyl)thio]phenoxy]ethyl]-,
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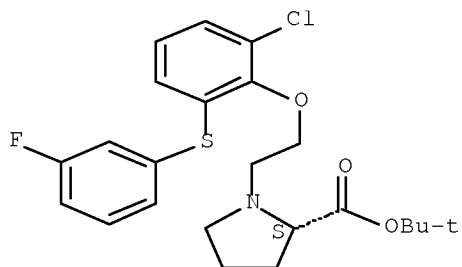
Absolute stereochemistry.



RN 905816-07-1 HCAPLUS

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1,1-dimethylethyl ester (CA INDEX NAME)

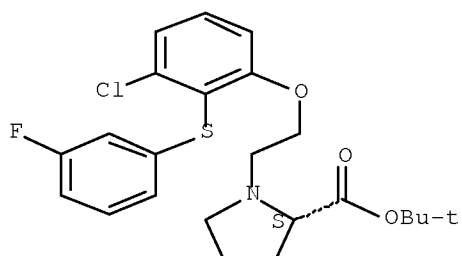
Absolute stereochemistry.



RN 905816-08-2 HCAPLUS

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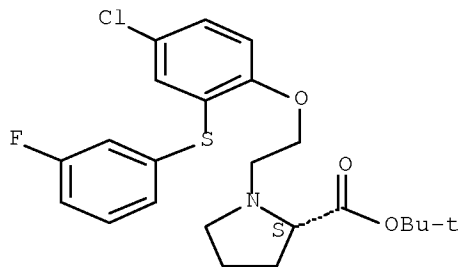
Absolute stereochemistry.



RN 905816-09-3 HCAPLUS

CN L-Proline, 1-[2-[4-chloro-2-[(3-fluorophenyl)thio]phenoxy]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:965214 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 141:411217

TITLE: A preparation of oxyphenyl and sulfanylphenyl

10/551737

derivatives of amino acids, useful as glycine transporter inhibitors

INVENTOR(S): Smith, Garrick Paul; Mikkelsen, Gitte; Andersen, Kim; Greve, Daniel Rodriguez; Eskildsen, Joergen

PATENT ASSIGNEE(S): H. Lundbeck A/S, Den.

SOURCE: PCT Int. Appl., 87 pp.

CODEN: PIXXD2

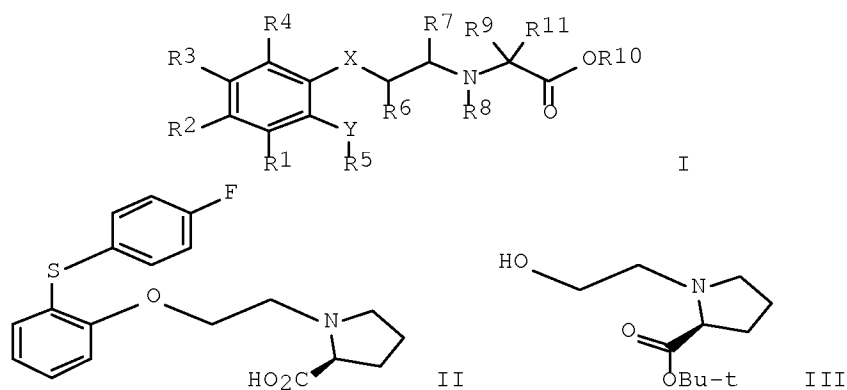
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

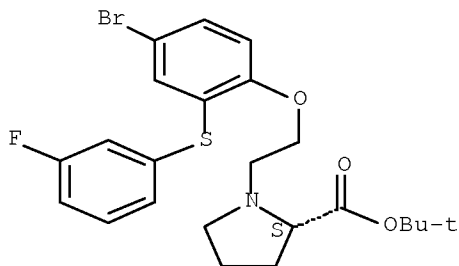
PATENT INFORMATION:

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WO 2004096761	A1	20041111	WO 2004-DK290	20040427
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AU 2004233942	A1	20041111	AU 2004-233942	20040427
CA 2523585	A1	20041111	CA 2004-2523585	20040427
EP 1622868	A1	20060208	EP 2004-729612	20040427
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
BR 2004009739	A	20060509	BR 2004-9739	20040427
CN 1780815	A	20060531	CN 2004-80011219	20040427
JP 2006524642	T	20061102	JP 2006-504368	20040427
MX 2005011198	A	20051214	MX 2005-11198	20051018
IN 2005CN02812	A	20070525	IN 2005-CN2812	20051031
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US 20060235003	A1	20061019	US 2006-551737	20060606 <--
PRIORITY APPLN. INFO.:			DK 2003-649	A 20030430
			US 2003-466755P	P 20030430
			WO 2004-DK290	W 20040427
OTHER SOURCE(S):			MARPAT 141:411217	
GI				



- AB The invention relates to a preparation of aromatic oxyphenyl and aromatic sulfanylphenyl derivs. of formula I [wherein: X is O, S, or CH₂, etc.; Y is O or S; R₁, R₂, R₃, and R₄ are independently selected from H, halogen, CN, NO₂, or alk(en/yn)yl, etc.; R₅ is (un)substituted aryl or monocyclic heteroaryl; R₆ is H, alk(en/yn)yl, cycloalk(en)yl, or alk(en/yn)ylsulfanyl, etc.; R₇ and R₈ are independently selected from H, alk(en/yn)yl, or cycloalk(en)yl; R₉ and R₁₁ are independently selected from H, alk(en/yn)yl, hydroxyalk(en/yn)yl, or alk(en/yn)ylsulfanyl, etc.; R₁₀ is H, alk(en/yn)yl, aryl, or arylalk(en/yn)yl, etc.; R₆ and R₈ together with the nitrogen may form 3-7 membered heterocyclic ring], useful as glycine transporter inhibitors (IC₅₀ < 10000 nM). The compds. of formula I are useful for the treatment of diseases such as schizophrenia, including both the pos. and the neg. symptoms of schizophrenia. For instance, pyrrolidinecarboxylic acid derivative II was prepared via etherification of 2-(3-fluorophenylsulfanyl)phenol by (hydroxyethyl)pyrrolidinecarboxylate derivative III.
- IT 791642-79-0P, (S)-1-[2-[4-Bromo-2-(3-fluorophenylsulfanyl)phenoxy]ethyl]pyrrolidine-2-carboxylic acid tert-butyl ester
- RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
- (intermediate; preparation of oxyphenyl and sulfanylphenyl derivs. of amino acids, useful as glycine transporter inhibitors)
- RN 791642-79-0 HCAPLUS
- CN L-Proline, 1-[2-[4-bromo-2-[(3-fluorophenyl)thio]phenoxy]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



IT 791642-81-4P, (S)-1-[2-[2-(4-Fluorophenylsulfanyl)phenoxy]ethyl]pyrrolidine-2-carboxylic acid
 791642-83-6P, (S)-1-[2-[2-(4-tert-Butylphenylsulfanyl)phenoxy]ethyl]pyrrolidine-2-carboxylic acid
 791642-84-7P, (S)-1-[2-[2-(4-Trifluoromethylphenylsulfanyl)phenoxy]ethyl]pyrrolidine-2-carboxylic acid
 791642-85-8P, (S)-1-[2-[2-(3-Fluorophenylsulfanyl)phenoxy]ethyl]pyrrolidine-2-carboxylic acid
 791642-86-9P, (S)-1-[2-[2-(4-Chlorophenylsulfanyl)-phenoxy]-ethyl]pyrrolidine-2-carboxylic acid 791642-87-0P, (S)-1-[2-[2-(3-Chlorophenylsulfanyl)phenoxy]ethyl]pyrrolidine-2-carboxylic acid 791642-88-1P, (S)-1-[2-[2-(3,4-Dichlorophenylsulfanyl)phenoxy]ethyl]pyrrolidine-2-carboxylic acid
 791642-90-5P, (S)-1-[2-[2-(3-Chloro-4-fluorophenylsulfanyl)phenoxy]ethyl]pyrrolidine-2-carboxylic acid
 791642-91-6P, (S)-1-[2-[2-(3-Chlorophenoxy)phenoxy]ethyl]pyrrolidine-2-carboxylic acid
 791642-92-7P 791642-93-8P 791642-94-9P
 791642-95-0P 791642-97-2P 791642-98-3P
 791642-99-4P 791643-00-0P 791643-01-1P
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 791643-29-3P, 2-[3-[2-(4-Trifluoromethylphenylsulfanyl)phenoxy]pyrrolidin-1-yl]propionic acid
 791643-30-6P, [[2-[2-(4-tert-Butylphenylsulfanyl)phenoxy]ethyl]-N-isopropylamino]acetic acid 791643-31-7P, [[2-[2-(4-tert-Butylphenylsulfanyl)phenoxy]ethyl]-N-methylamino]acetic acid 791643-33-9P, [[2-[2-(3,4-Dichlorophenylsulfanyl)phenoxy]ethyl]-N-methylamino]acetic acid
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 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

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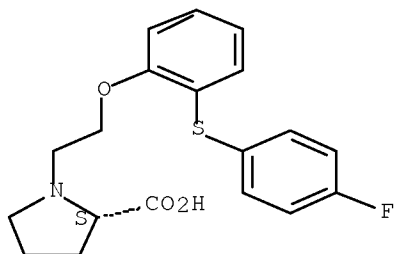
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)

(preparation of oxyphenyl and sulfanylphenyl derivs. of amino acids, useful
as glycine transporter inhibitors)

RN 791642-81-4 HCAPLUS

CN L-Proline, 1-[2-[2-[(4-fluorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

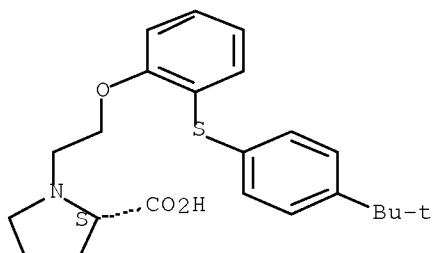
Absolute stereochemistry.



RN 791642-83-6 HCAPLUS

CN L-Proline, 1-[2-[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]ethyl]- (CA INDEX NAME)

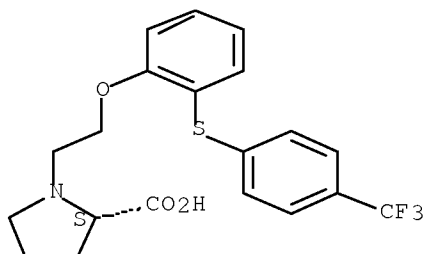
Absolute stereochemistry.



RN 791642-84-7 HCAPLUS

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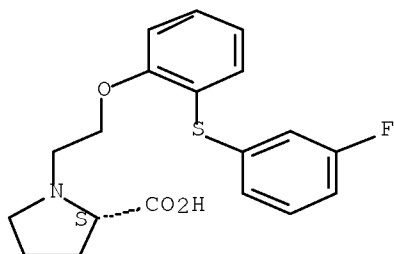
Absolute stereochemistry.



RN 791642-85-8 HCAPLUS

CN L-Proline, 1-[2-[2-[(3-fluorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

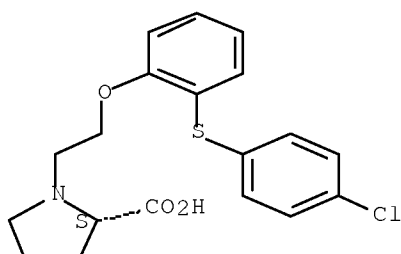
Absolute stereochemistry.



RN 791642-86-9 HCAPLUS

CN L-Proline, 1-[2-[2-[(4-chlorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

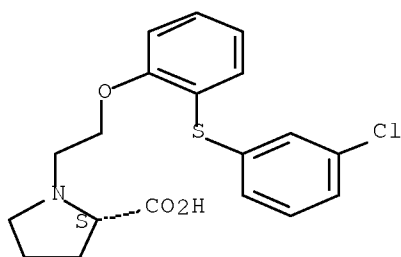
Absolute stereochemistry.



RN 791642-87-0 HCAPLUS

CN L-Proline, 1-[2-[2-[(3-chlorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



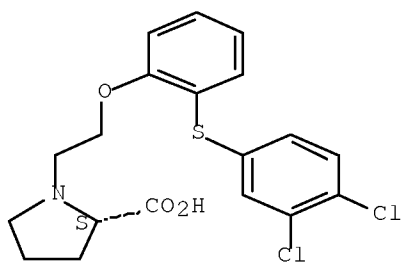
RN 791642-88-1 HCAPLUS

CN L-Proline, 1-[2-[2-[(3,4-dichlorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

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NAME)

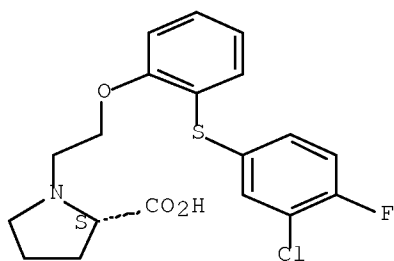
Absolute stereochemistry.



RN 791642-90-5 HCAPLUS

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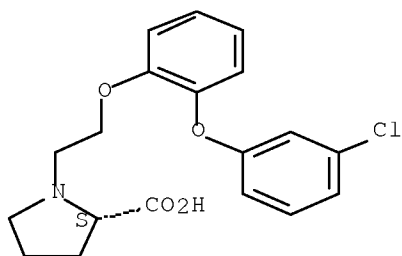
Absolute stereochemistry.



RN 791642-91-6 HCAPLUS

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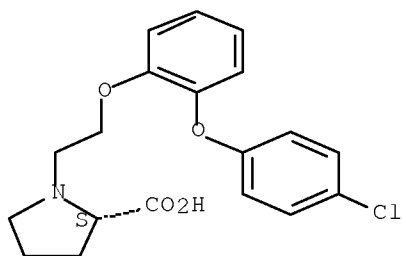
Absolute stereochemistry.



RN 791642-92-7 HCAPLUS

CN L-Proline, 1-[2-[2-(4-chlorophenoxy)phenoxy]ethyl]- (CA INDEX NAME)

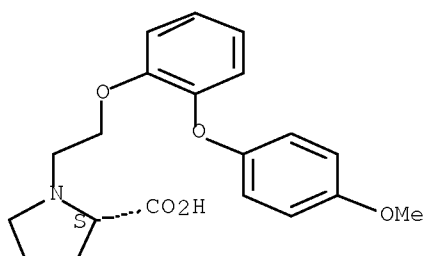
Absolute stereochemistry.



RN 791642-93-8 HCAPLUS

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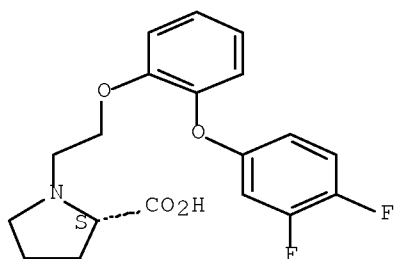
Absolute stereochemistry.



RN 791642-94-9 HCAPLUS

CN L-Proline, 1-[2-[2-(3,4-difluorophenoxy)phenoxy]ethyl]- (CA INDEX NAME)

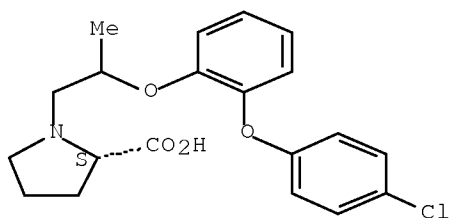
Absolute stereochemistry.



RN 791642-95-0 HCAPLUS

CN L-Proline, 1-[2-[2-(4-chlorophenoxy)phenoxy]propyl]- (CA INDEX NAME)

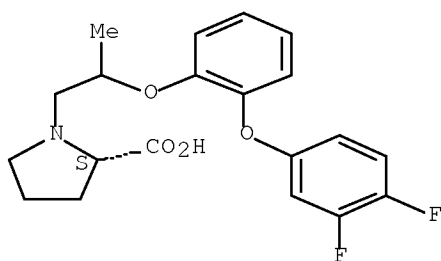
Absolute stereochemistry.



RN 791642-97-2 HCAPLUS

CN L-Proline, 1-[2-[2-(3,4-difluorophenoxy)phenoxy]propyl]- (CA INDEX NAME)

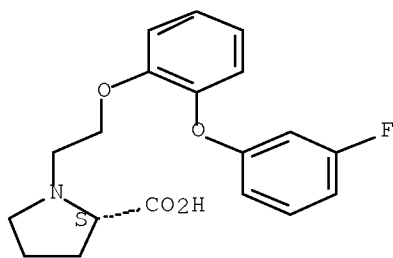
Absolute stereochemistry.



RN 791642-98-3 HCAPLUS

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Absolute stereochemistry.

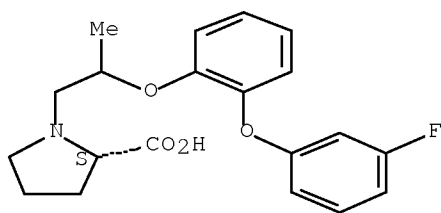


RN 791642-99-4 HCAPLUS

CN L-Proline, 1-[2-[2-(3-fluorophenoxy)phenoxy]propyl]- (CA INDEX NAME)

Absolute stereochemistry.

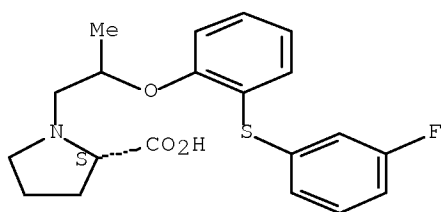
10/551737



RN 791643-00-0 HCAPLUS

CN L-Proline, 1-[2-[2-[(3-fluorophenyl)thio]phenoxy]propyl]- (CA INDEX NAME)

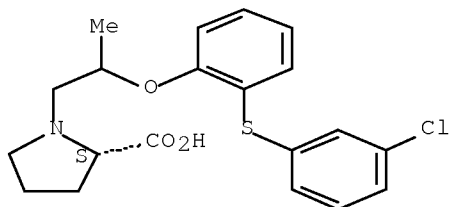
Absolute stereochemistry.



RN 791643-01-1 HCAPLUS

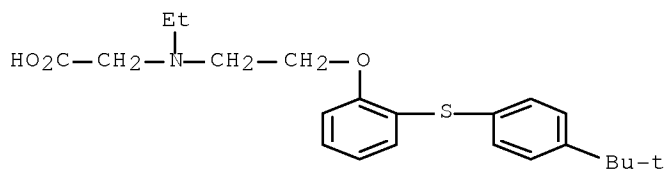
CN L-Proline, 1-[2-[2-[(3-chlorophenyl)thio]phenoxy]propyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 791643-02-2 HCAPLUS

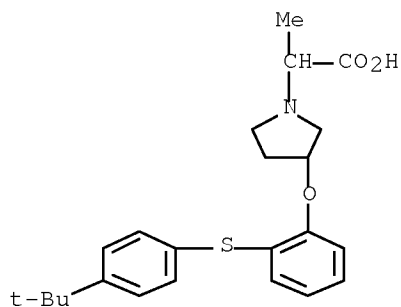
CN Glycine, N-[2-[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]ethyl]-N-ethyl- (CA INDEX NAME)



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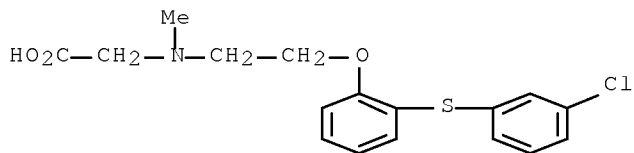
RN 791643-04-4 HCAPLUS

CN 1-Pyrrolidineacetic acid, 3-[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]-
 α -methyl- (CA INDEX NAME)



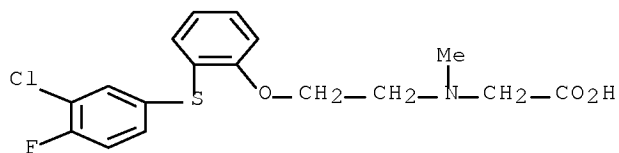
RN 791643-06-6 HCAPLUS

CN Glycine, N-[2-[2-[(3-chlorophenyl)thio]phenoxy]ethyl]-N-methyl- (CA INDEX NAME)



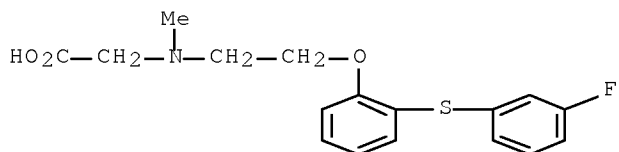
RN 791643-08-8 HCAPLUS

CN Glycine, N-[2-[2-[(3-chloro-4-fluorophenyl)thio]phenoxy]ethyl]-N-methyl- (CA INDEX NAME)



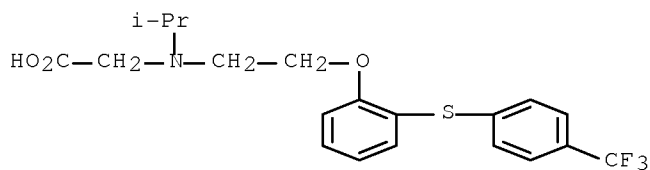
RN 791643-10-2 HCAPLUS

CN Glycine, N-[2-[2-[(3-fluorophenyl)thio]phenoxy]ethyl]-N-methyl- (CA INDEX NAME)



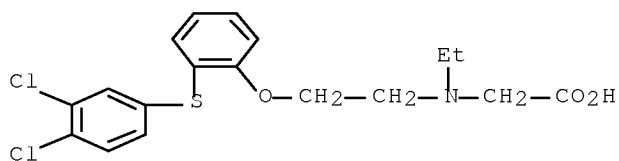
RN 791643-12-4 HCAPLUS

CN Glycine, N-(1-methylethyl)-N-[2-[2-[[4-(trifluoromethyl)phenyl]thio]phenoxy]ethyl]- (CA INDEX NAME)



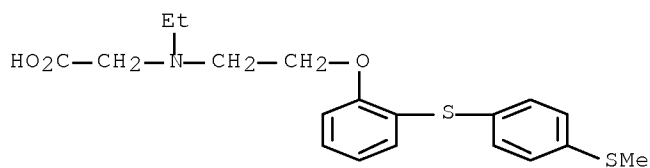
RN 791643-14-6 HCAPLUS

CN Glycine, N-[2-[2-[(3,4-dichlorophenyl)thio]phenoxy]ethyl]-N-ethyl- (CA INDEX NAME)



RN 791643-16-8 HCAPLUS

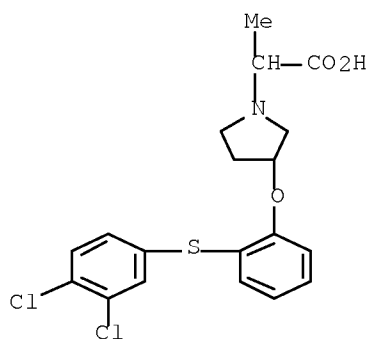
CN Glycine, N-ethyl-N-[2-[2-[[4-(methylthio)phenyl]thio]phenoxy]ethyl]- (CA INDEX NAME)



RN 791643-17-9 HCAPLUS

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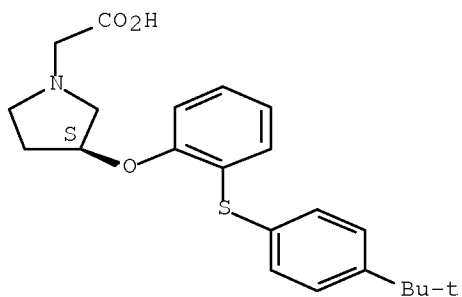
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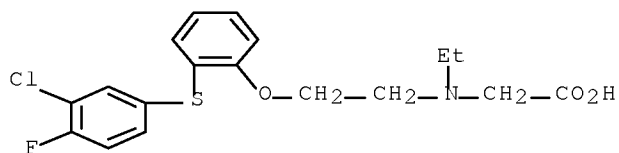
CN 1-Pyrrolidineacetic acid, 3-[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 791643-20-4 HCAPLUS

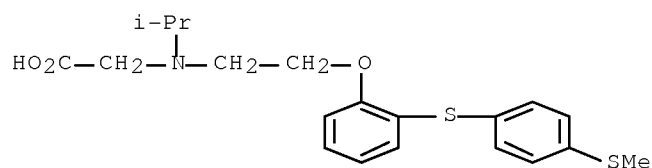
CN Glycine, N-[2-[2-[(3-chloro-4-fluorophenyl)thio]phenoxy]ethyl]-N-ethyl- (CA INDEX NAME)



RN 791643-21-5 HCAPLUS

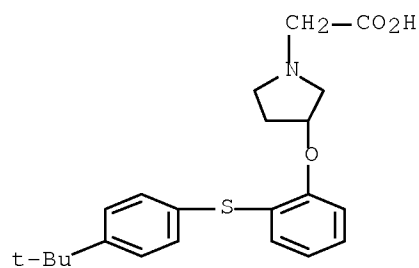
CN Glycine, N-(1-methylethyl)-N-[2-[2-[[4-(methylthio)phenyl]thio]phenoxy]ethyl]- (CA INDEX NAME)

10/551737



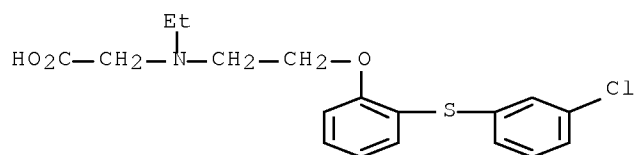
RN 791643-22-6 HCAPLUS

CN 1-Pyrrolidineacetic acid, 3-[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]-
(CA INDEX NAME)



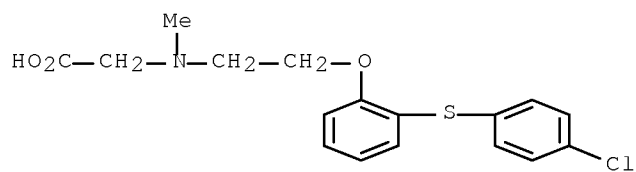
RN 791643-25-9 HCAPLUS

CN Glycine, N-[2-[2-[(3-chlorophenyl)thio]phenoxy]ethyl]-N-ethyl- (CA INDEX
NAME)



RN 791643-27-1 HCAPLUS

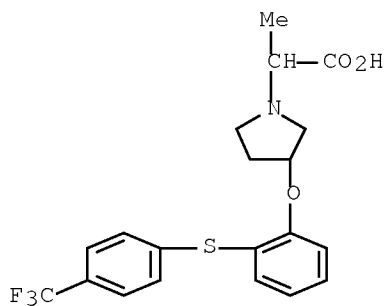
CN Glycine, N-[2-[2-[(4-chlorophenyl)thio]phenoxy]ethyl]-N-methyl- (CA INDEX
NAME)



RN 791643-29-3 HCAPLUS

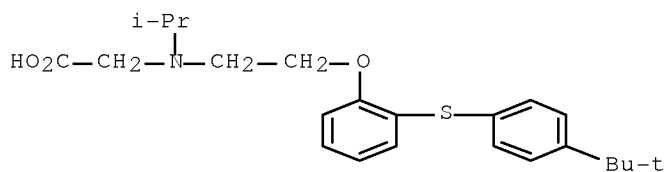
10/551737

CN 1-Pyrrolidineacetic acid, α -methyl-3-[2-[[4-(trifluoromethyl)phenyl]thio]phenoxy]- (CA INDEX NAME)



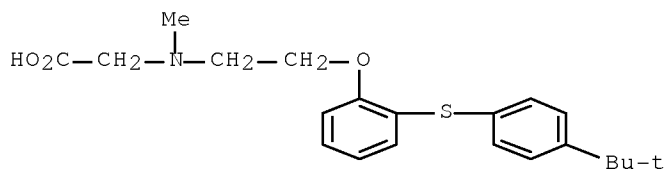
RN 791643-30-6 HCAPLUS

CN Glycine, N-[2-[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]ethyl]-N-(1-methylethyl)- (CA INDEX NAME)



RN 791643-31-7 HCAPLUS

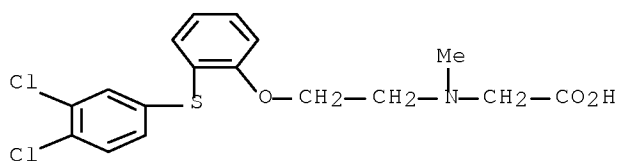
CN Glycine, N-[2-[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]ethyl]-N-methyl- (CA INDEX NAME)



RN 791643-33-9 HCAPLUS

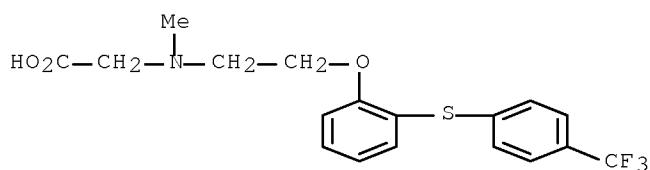
CN Glycine, N-[2-[2-[(3,4-dichlorophenyl)thio]phenoxy]ethyl]-N-methyl- (CA INDEX NAME)

10/551737



RN 791643-34-0 HCAPLUS

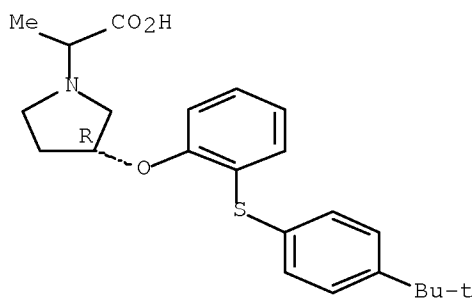
CN Glycine, N-methyl-N-[2-[2-[[4-(trifluoromethyl)phenyl]thio]phenoxy]ethyl]-
(CA INDEX NAME)



RN 791643-35-1 HCAPLUS

CN 1-Pyrrolidineacetic acid, 3-[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]-
α-methyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.

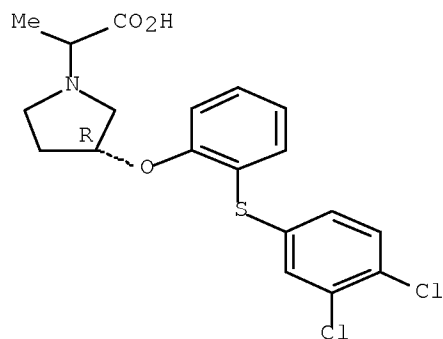


RN 791643-37-3 HCAPLUS

CN 1-Pyrrolidineacetic acid, 3-[2-[(3,4-dichlorophenyl)thio]phenoxy]-α-
methyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.

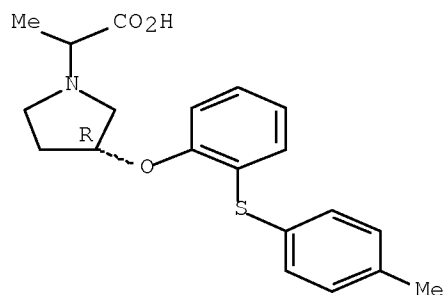
10/551737



RN 791643-38-4 HCAPLUS

CN 1-Pyrrolidineacetic acid, α -methyl-3-[2-[(4-methylphenyl)thio]phenoxy]-, (3R)- (CA INDEX NAME)

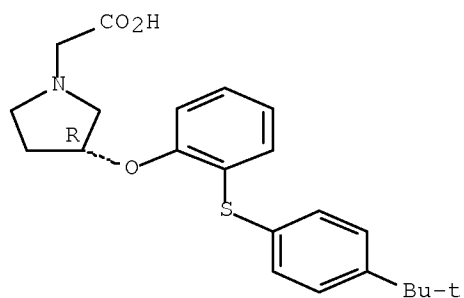
Absolute stereochemistry.



RN 791643-39-5 HCAPLUS

CN 1-Pyrrolidineacetic acid, 3-[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]-, (3R)- (CA INDEX NAME)

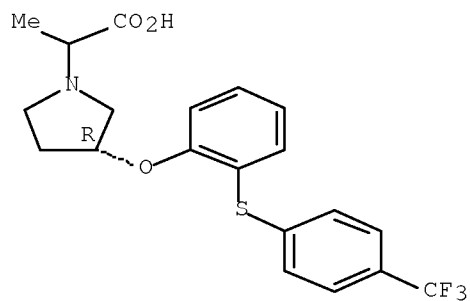
Absolute stereochemistry.



RN 791643-41-9 HCAPLUS

CN 1-Pyrrolidineacetic acid, α -methyl-3-[2-[[4-(trifluoromethyl)phenyl]thio]phenoxy]-, (3R)- (CA INDEX NAME)

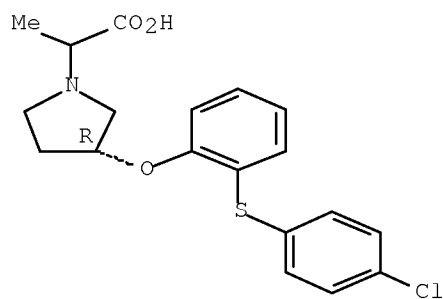
Absolute stereochemistry.



RN 791643-42-0 HCAPLUS

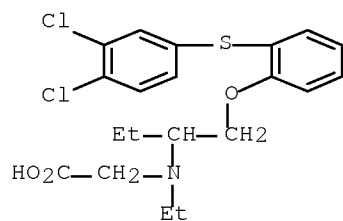
CN 1-Pyrrolidineacetic acid, 3-[2-[(4-chlorophenyl)thio]phenoxy]-α-methyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 791643-45-3 HCAPLUS

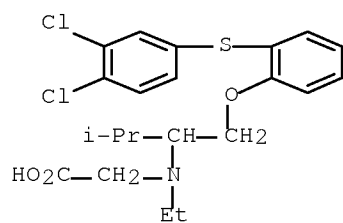
CN Glycine, N-[1-[[2-[(3,4-dichlorophenyl)thio]phenoxy]methyl]propyl]-N-ethyl- (CA INDEX NAME)



RN 791643-46-4 HCAPLUS

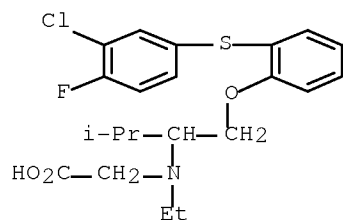
CN Glycine, N-[1-[[2-[(3,4-dichlorophenyl)thio]phenoxy]methyl]-2-methylpropyl]-N-ethyl- (CA INDEX NAME)

10/551737



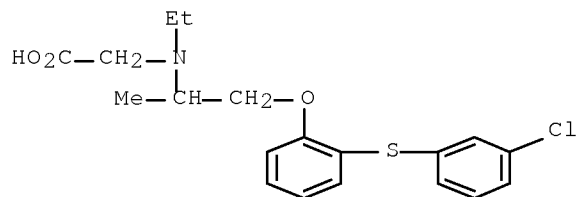
RN 791643-48-6 HCAPLUS

CN Glycine, N-[1-[[2-[(3-chloro-4-fluorophenyl)thio]phenoxy]methyl]-2-methylpropyl]-N-ethyl- (CA INDEX NAME)



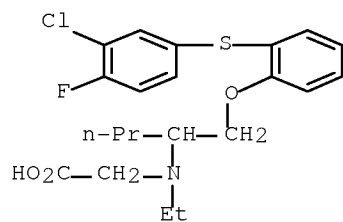
RN 791643-49-7 HCAPLUS

CN Glycine, N-[2-[2-[(3-chlorophenyl)thio]phenoxy]-1-methylethyl]-N-ethyl- (CA INDEX NAME)



RN 791643-51-1 HCAPLUS

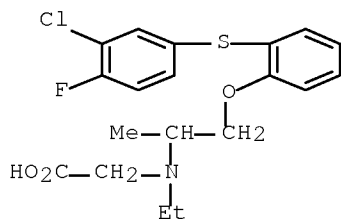
CN Glycine, N-[1-[[2-[(3-chloro-4-fluorophenyl)thio]phenoxy]methyl]butyl]-N-ethyl- (CA INDEX NAME)



10/551737

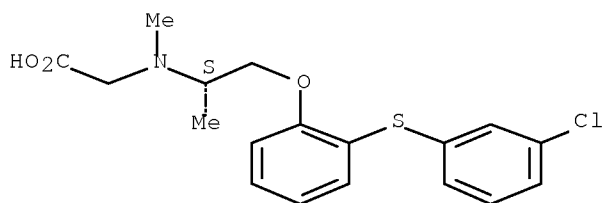
RN 791643-52-2 HCAPLUS

CN Glycine, N-[2-[2-[(3-chloro-4-fluorophenyl)thio]phenoxy]-1-methylethyl]-N-ethyl- (CA INDEX NAME)



RN 791643-53-3 HCAPLUS

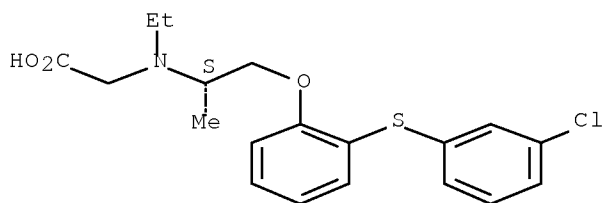
CN Glycine, N-[(1S)-2-[2-[(3-chlorophenyl)thio]phenoxy]-1-methylethyl]-N-methyl- (CA INDEX NAME)



RN 791643-55-5 HCAPLUS

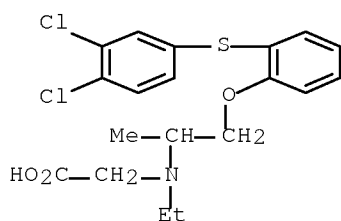
CN Glycine, N-[(1S)-2-[2-[(3-chlorophenyl)thio]phenoxy]-1-methylethyl]-N-ethyl- (CA INDEX NAME)

Absolute stereochemistry.



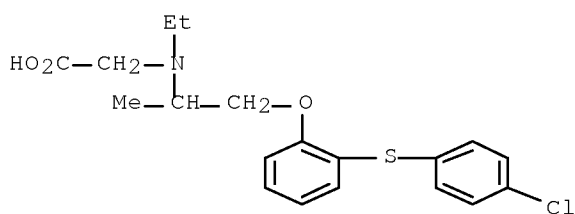
RN 791643-57-7 HCAPLUS

CN Glycine, N-[2-[2-[(3,4-dichlorophenyl)thio]phenoxy]-1-methylethyl]-N-ethyl- (CA INDEX NAME)



RN 791643-58-8 HCAPLUS

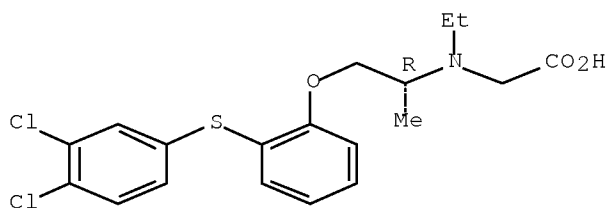
CN Glycine, N-[2-[2-[(4-chlorophenyl)thio]phenoxy]-1-methylethyl]-N-ethyl-
(CA INDEX NAME)



RN 791643-63-5 HCAPLUS

CN Glycine, N-[(1R)-2-[2-[(3,4-dichlorophenyl)thio]phenoxy]-1-methylethyl]-N-ethyl-
(CA INDEX NAME)

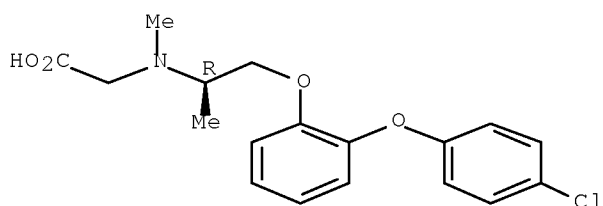
Absolute stereochemistry.



RN 791643-65-7 HCAPLUS

CN Glycine, N-[(1R)-2-[2-(4-chlorophenoxy)phenoxy]-1-methylethyl]-N-methyl-
(CA INDEX NAME)

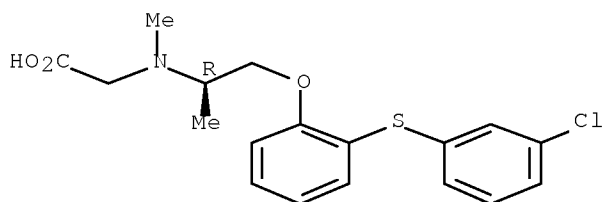
Absolute stereochemistry.



RN 791643-66-8 HCAPLUS

CN Glycine, N-[(1R)-2-[2-[(3-chlorophenyl)thio]phenoxy]-1-methylethyl]-N-methyl- (CA INDEX NAME)

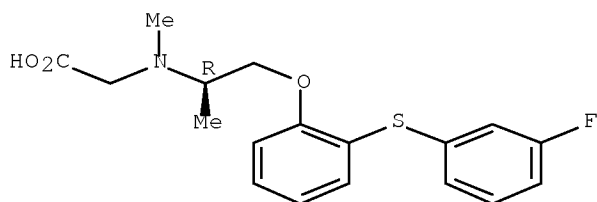
Absolute stereochemistry.



RN 791643-68-0 HCAPLUS

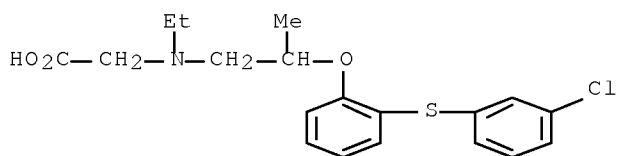
CN Glycine, N-[(1R)-2-[2-[(3-fluorophenyl)thio]phenoxy]-1-methylethyl]-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.



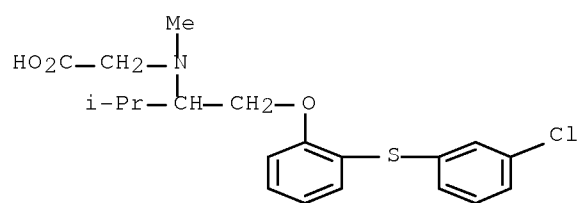
RN 791643-70-4 HCAPLUS

CN Glycine, N-[2-[2-[(3-chlorophenyl)thio]phenoxy]propyl]-N-ethyl- (CA INDEX NAME)



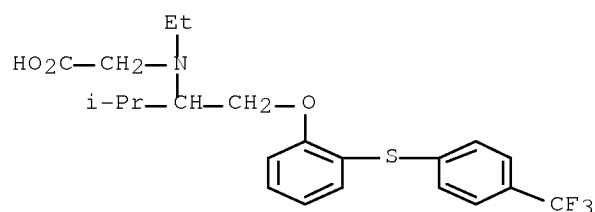
RN 791643-71-5 HCAPLUS

CN Glycine, N-[1-[[2-[(3-chlorophenyl)thio]phenoxy]methyl]-2-methylpropyl]-N-methyl- (CA INDEX NAME)



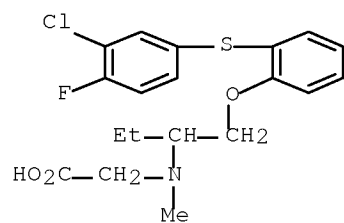
RN 791643-72-6 HCAPLUS

CN Glycine, N-ethyl-N-[2-methyl-1-[[2-[[4-(trifluoromethyl)phenyl]thio]phenoxy]methyl]propyl]- (CA INDEX NAME)



RN 791643-73-7 HCAPLUS

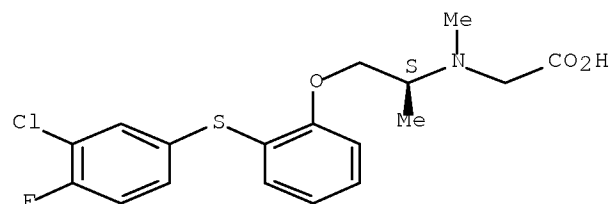
CN Glycine, N-[1-[[2-[(3-chloro-4-fluorophenyl)thio]phenoxy]methyl]propyl]-N-methyl- (CA INDEX NAME)



RN 791643-74-8 HCAPLUS

CN Glycine, N-[(1S)-2-[2-[(3-chloro-4-fluorophenyl)thio]phenoxy]-1-methylethyl]-N-methyl- (CA INDEX NAME)

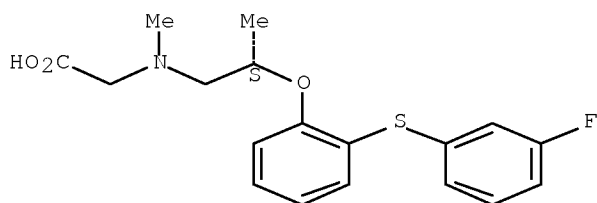
Absolute stereochemistry.



RN 791643-75-9 HCAPLUS

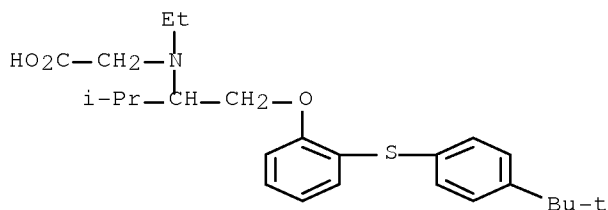
CN Glycine, N-[(2S)-2-[2-[(3-fluorophenyl)thio]phenoxy]propyl]-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.



RN 791643-76-0 HCAPLUS

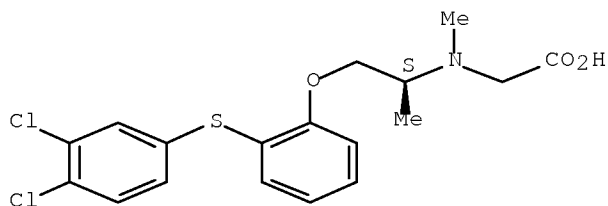
CN Glycine, N-[1-[[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]methyl]-2-methylpropyl]-N-ethyl- (CA INDEX NAME)



RN 791643-77-1 HCAPLUS

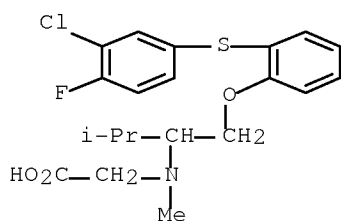
CN Glycine, N-[(1S)-2-[2-[(3,4-dichlorophenyl)thio]phenoxy]-1-methylethyl]-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.



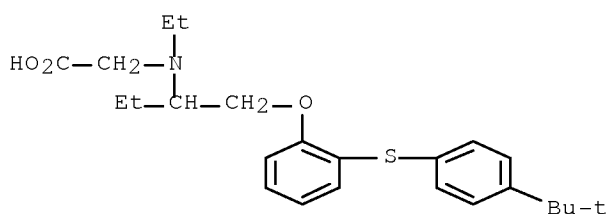
RN 791643-78-2 HCAPLUS

CN Glycine, N-[1-[[2-[(3-chloro-4-fluorophenyl)thio]phenoxy]methyl]-2-methylpropyl]-N-methyl- (CA INDEX NAME)



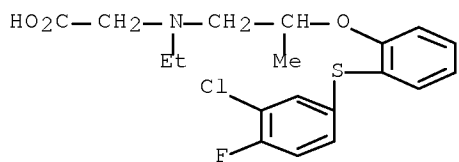
RN 791643-79-3 HCAPLUS

CN Glycine, N-[1-[[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]methyl]propyl]-N-ethyl- (CA INDEX NAME)



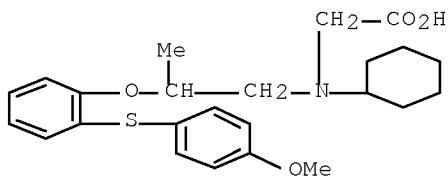
RN 791643-80-6 HCAPLUS

CN Glycine, N-[2-[[2-[[3-chloro-4-fluorophenyl]thio]phenoxy]propyl]-N-ethyl- (CA INDEX NAME)



RN 791643-81-7 HCAPLUS

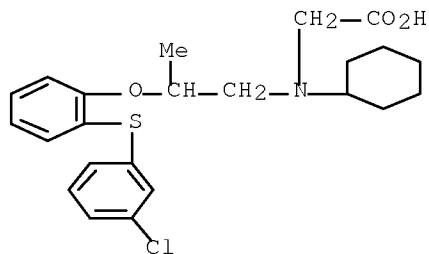
CN Glycine, N-cyclohexyl-N-[2-[[2-[[4-methoxyphenyl]thio]phenoxy]propyl]- (CA INDEX NAME)



RN 791643-84-0 HCAPLUS

CN Glycine, N-[2-[[2-[[3-chlorophenyl]thio]phenoxy]propyl]-N-cyclohexyl- (CA

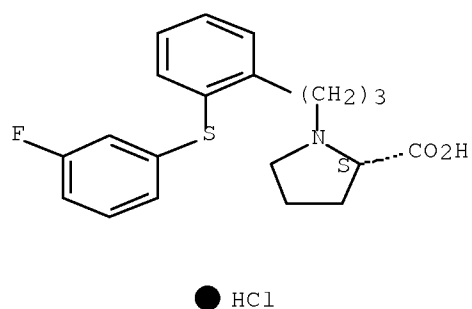
INDEX NAME)



RN 791643-85-1 HCAPLUS

CN L-Proline, 1-[3-[2-[(3-fluorophenyl)thio]phenyl]propyl]-, hydrochloride
(9CI) (CA INDEX NAME)

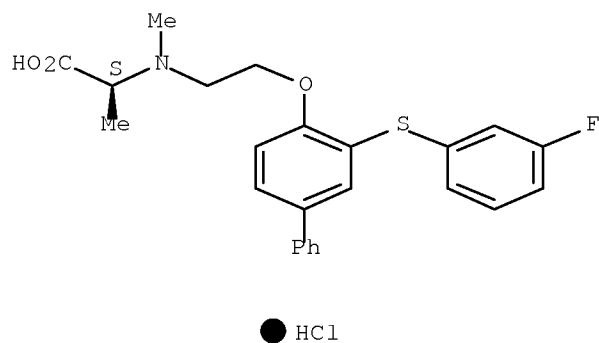
Absolute stereochemistry.



RN 791643-86-2 HCAPLUS

CN L-Alanine, N-[2-[[3-[(3-fluorophenyl)thio][1,1'-biphenyl]-4-yl]oxy]ethyl]-
N-methyl-, hydrochloride (9CI) (CA INDEX NAME)

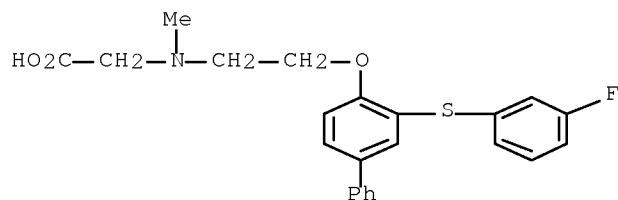
Absolute stereochemistry.



RN 791643-87-3 HCAPLUS

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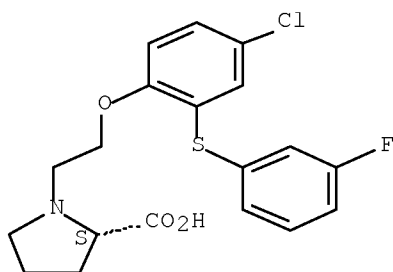
CN Glycine, N-[2-[[3-[(3-fluorophenyl)thio][1,1'-biphenyl]-4-yl]oxy]ethyl]-N-methyl- (CA INDEX NAME)



RN 791643-88-4 HCAPLUS

CN L-Proline, 1-[2-[4-chloro-2-[(3-fluorophenyl)thio]phenoxy]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

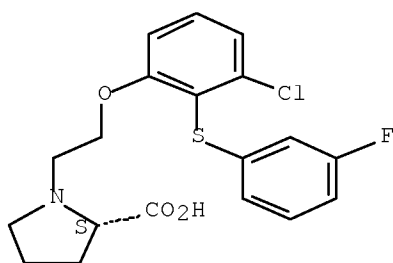


● HCl

RN 791643-90-8 HCAPLUS

CN L-Proline, 1-[2-[3-chloro-2-[(3-fluorophenyl)thio]phenoxy]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



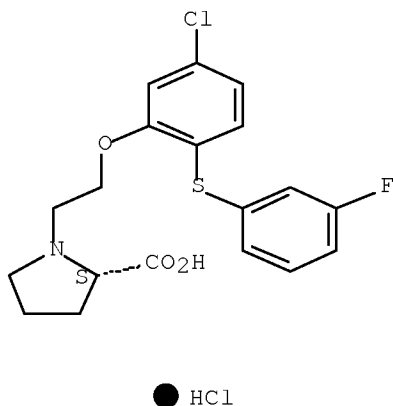
● HCl

10/551737

RN 791643-91-9 HCAPLUS

CN L-Proline, 1-[2-[5-chloro-2-[(3-fluorophenyl)thio]phenoxy]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

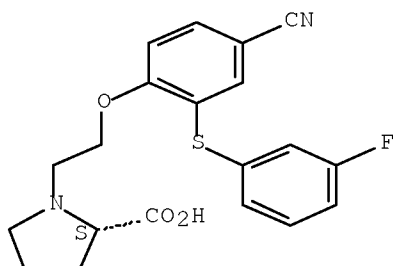
Absolute stereochemistry.



RN 791643-92-0 HCAPLUS

CN L-Proline, 1-[2-[4-cyano-2-[(3-fluorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.

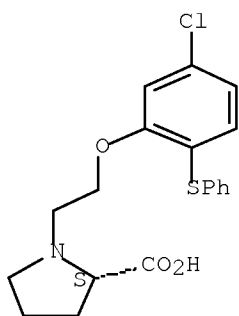


RN 791643-94-2 HCAPLUS

CN L-Proline, 1-[2-[5-chloro-2-(phenylthio)phenoxy]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/551737

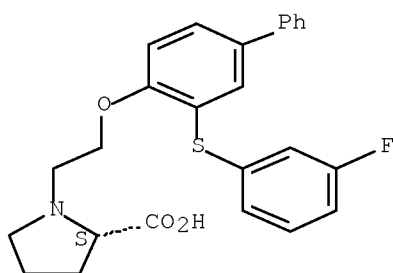


● HCl

RN 791643-95-3 HCAPLUS

CN L-Proline, 1-[2-[[3-[(3-fluorophenyl)thio][1,1'-biphenyl]-4-yl]oxy]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



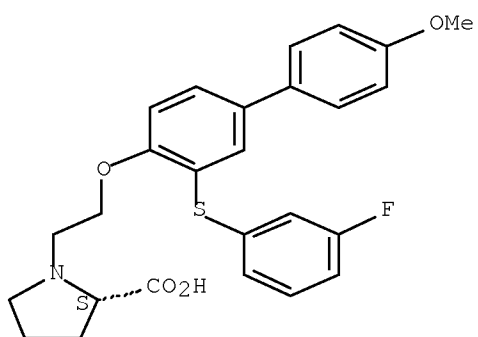
● HCl

RN 791643-97-5 HCAPLUS

CN L-Proline, 1-[2-[[3-[(3-fluorophenyl)thio]-4'-methoxy[1,1'-biphenyl]-4-yl]oxy]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/551737

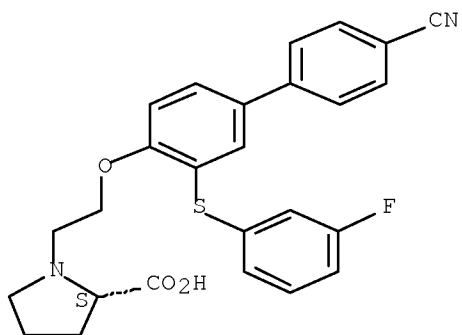


● HCl

RN 791643-99-7 HCAPLUS

CN L-Proline, 1-[2-[[4'-cyano-3-[(3-fluorophenyl)thio][1,1'-biphenyl]-4-yl]oxy]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



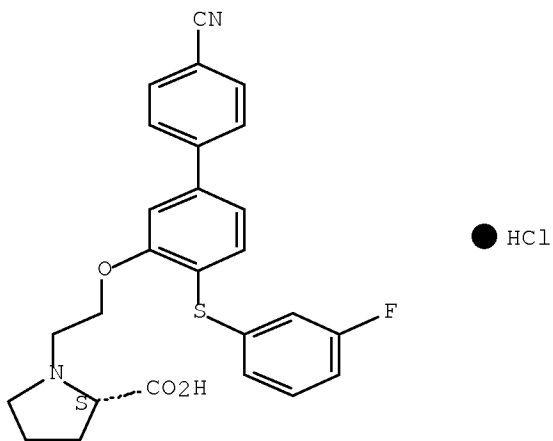
● HCl

RN 791644-00-3 HCAPLUS

CN L-Proline, 1-[2-[[4'-cyano-4-[(3-fluorophenyl)thio][1,1'-biphenyl]-3-yl]oxy]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

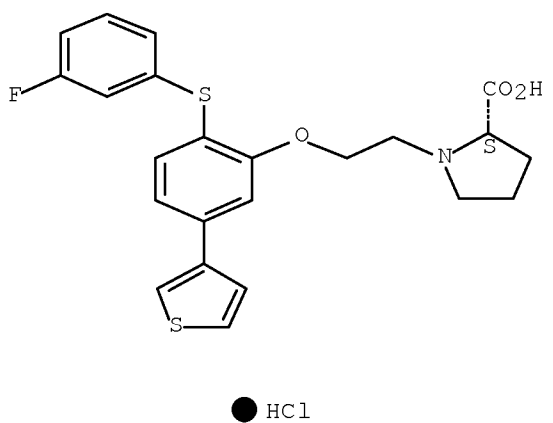
10/551737



RN 791644-02-5 HCAPLUS

CN L-Proline, 1-[2-[2-[(3-fluorophenyl)thio]-5-(3-thienyl)phenoxy]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

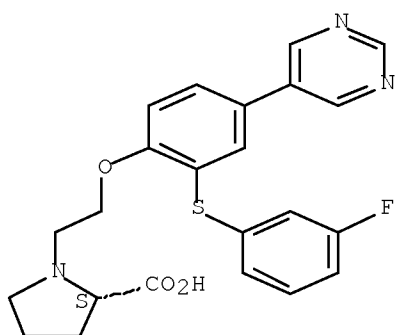


RN 791644-04-7 HCAPLUS

CN L-Proline, 1-[2-[2-[(3-fluorophenyl)thio]-4-(5-pyrimidinyl)phenoxy]ethyl]-
, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/551737

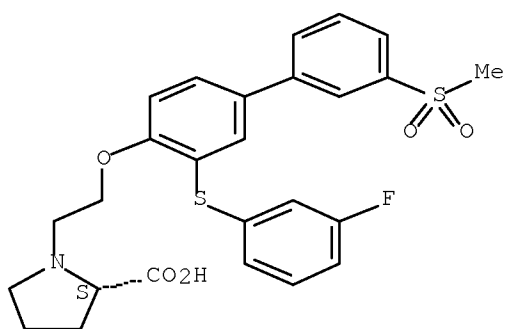


● HCl

RN 791644-06-9 HCAPLUS

CN L-Proline, 1-[2-[[3-[(3-fluorophenyl)thio]-3'-(methoxysulfonyl)[1,1'-biphenyl]-4-yl]oxy]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



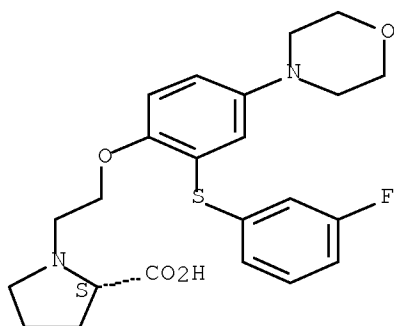
● HCl

RN 791644-08-1 HCAPLUS

CN L-Proline, 1-[2-[2-[(3-fluorophenyl)thio]-4-(4-morpholinyl)phenoxy]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/551737

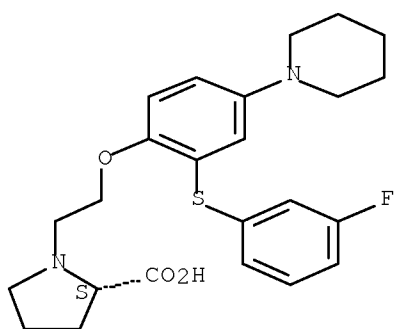


● HCl

RN 791644-09-2 HCAPLUS

CN L-Proline, 1-[2-[2-[(3-fluorophenyl)thio]-4-(1-piperidinyl)phenoxy]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

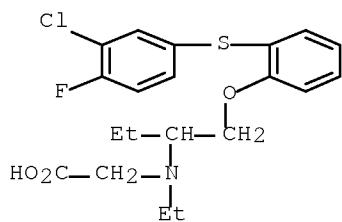
Absolute stereochemistry.



● HCl

RN 791644-10-5 HCAPLUS

CN Glycine, N-[1-[[2-[(3-chloro-4-fluorophenyl)thio]phenoxy]methyl]propyl]-N-ethyl- (CA INDEX NAME)

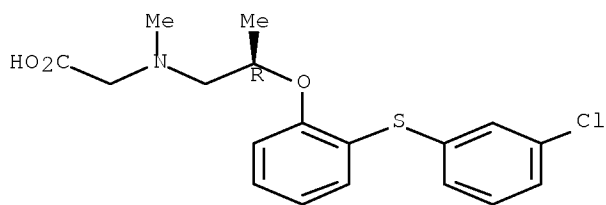


10/551737

RN 791644-11-6 HCAPLUS

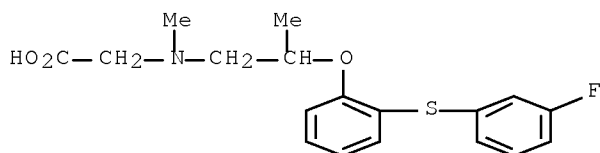
CN Glycine, N-[(2R)-2-[2-[(3-chlorophenyl)thio]phenoxy]propyl]-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.



RN 791644-12-7 HCAPLUS

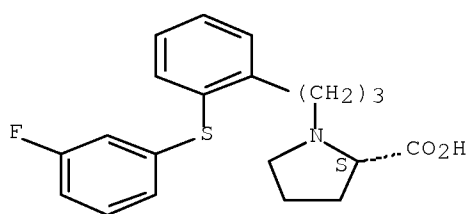
CN Glycine, N-[2-[2-[(3-fluorophenyl)thio]phenoxy]propyl]-N-methyl- (CA INDEX NAME)



RN 791644-15-0 HCAPLUS

CN L-Proline, 1-[3-[2-[(3-fluorophenyl)thio]phenyl]propyl]- (CA INDEX NAME)

Absolute stereochemistry.

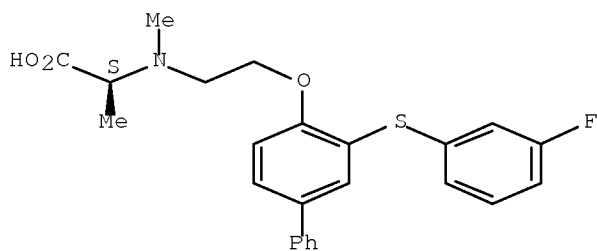


RN 791644-16-1 HCAPLUS

CN L-Alanine, N-[2-[[3-[(3-fluorophenyl)thio][1,1'-biphenyl]-4-yl]oxy]ethyl]-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.

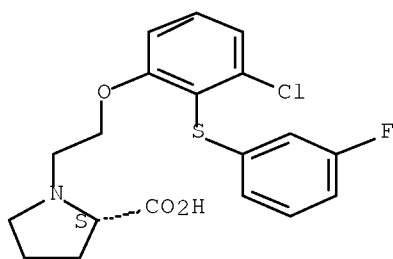
10/551737



RN 791644-17-2 HCAPLUS

CN L-Proline, 1-[2-[3-chloro-2-[(3-fluorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

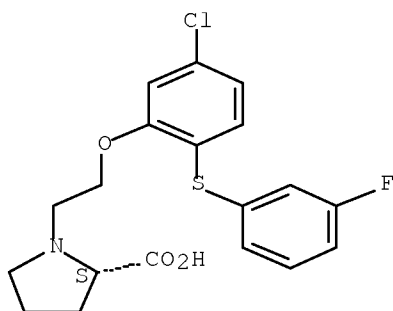
Absolute stereochemistry.



RN 791644-18-3 HCAPLUS

CN L-Proline, 1-[2-[5-chloro-2-[(3-fluorophenyl)thio]phenoxy]ethyl]- (CA INDEX NAME)

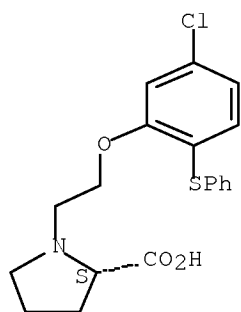
Absolute stereochemistry.



RN 791644-19-4 HCAPLUS

CN L-Proline, 1-[2-[5-chloro-2-(phenylthio)phenoxy]ethyl]- (CA INDEX NAME)

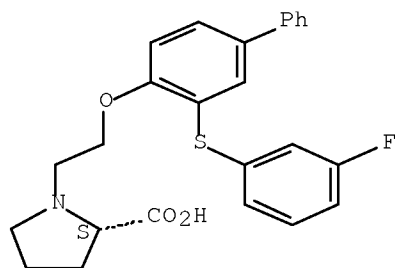
Absolute stereochemistry.



RN 791644-20-7 HCAPLUS

CN L-Proline, 1-[2-[3-[3-(3-fluorophenyl)thio][1,1'-biphenyl]-4-yl]oxy]ethyl]-
(CA INDEX NAME)

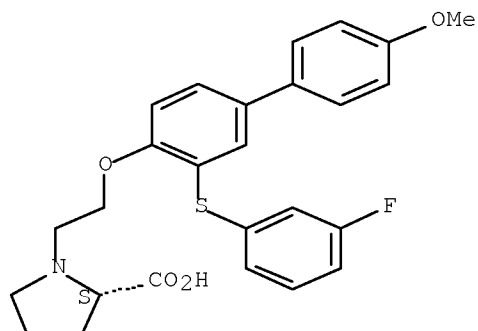
Absolute stereochemistry.



RN 791644-21-8 HCAPLUS

CN L-Proline, 1-[2-[3-[3-(3-fluorophenyl)thio]-4'-methoxy[1,1'-biphenyl]-4-yl]oxy]ethyl]-
(CA INDEX NAME)

Absolute stereochemistry.

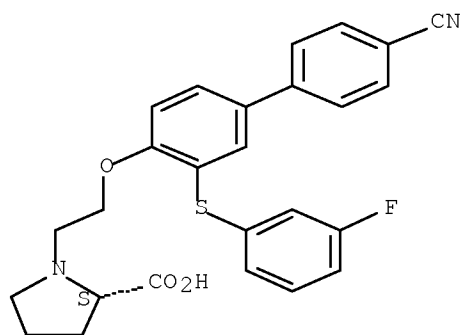


RN 791644-22-9 HCAPLUS

CN L-Proline, 1-[2-[4'-cyano-3-[3-(3-fluorophenyl)thio][1,1'-biphenyl]-4-yl]oxy]ethyl]-
(CA INDEX NAME)

10/551737

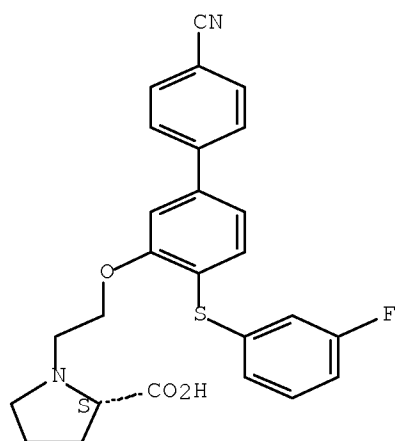
Absolute stereochemistry.



RN 791644-23-0 HCAPLUS

CN L-Proline, 1-[2-[[4'-cyano-4-[(3-fluorophenyl)thio][1,1'-biphenyl]-3-yl]oxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.

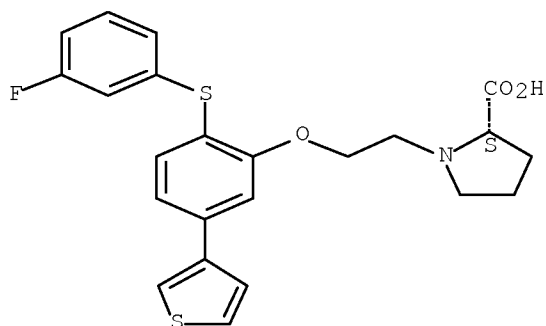


RN 791644-24-1 HCAPLUS

CN L-Proline, 1-[2-[2-[(3-fluorophenyl)thio]-5-(3-thienyl)phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.

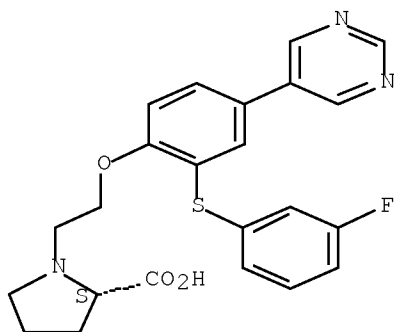
10/551737



RN 791644-25-2 HCAPLUS

CN L-Proline, 1-[2-[2-[(3-fluorophenyl)thio]-4-(5-pyrimidinyl)phenoxy]ethyl]-
(CA INDEX NAME)

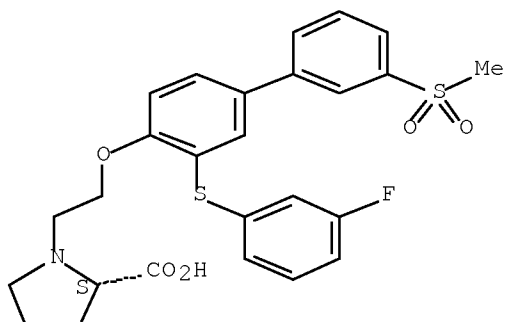
Absolute stereochemistry.



RN 791644-26-3 HCAPLUS

CN L-Proline, 1-[2-[3-[(3-fluorophenyl)thio]-3'-(methylsulfonyl)[1,1'-
biphenyl]-4-yl]oxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.

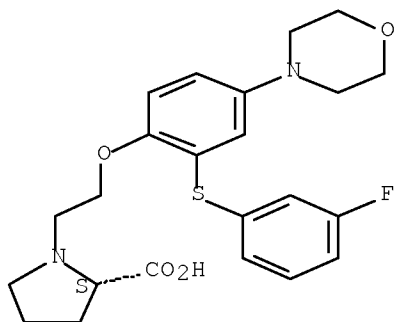


RN 791644-27-4 HCAPLUS

10/551737

CN L-Proline, 1-[2-[2-[(3-fluorophenyl)thio]-4-(4-morpholinyl)phenoxy]ethyl]-
(CA INDEX NAME)

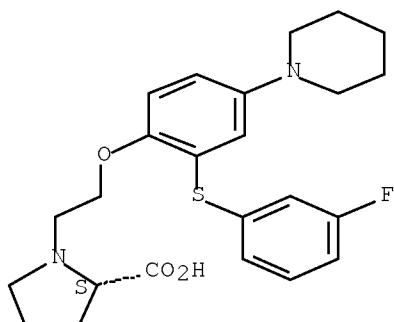
Absolute stereochemistry.



RN 791644-28-5 HCAPLUS

CN L-Proline, 1-[2-[2-[(3-fluorophenyl)thio]-4-(1-piperidiny)phenoxy]ethyl]-
(CA INDEX NAME)

Absolute stereochemistry.



IT 791643-98-6 791644-01-4 791644-07-0

RL: RCT (Reactant); RACT (Reactant or reagent)

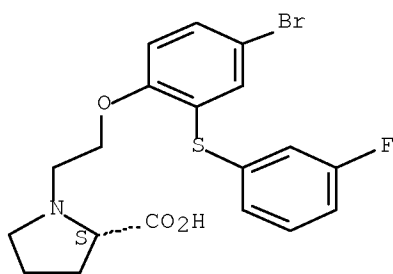
(reactant; preparation of oxyphenyl and sulfanylphenyl derivs. of amino acids, useful as glycine transporter inhibitors)

RN 791643-98-6 HCAPLUS

CN L-Proline, 1-[2-[4-bromo-2-[(3-fluorophenyl)thio]phenoxy]ethyl]-,
hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/551737

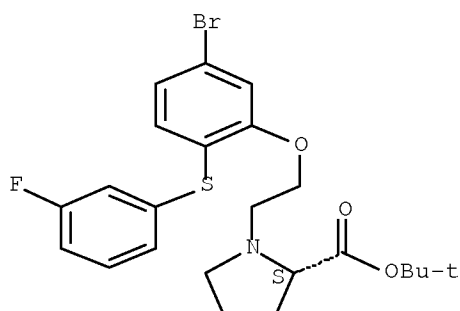


● HCl

RN 791644-01-4 HCAPLUS

CN L-Proline, 1-[2-[5-bromo-2-[(3-fluorophenyl)thio]phenoxy]ethyl]-,
1,1-dimethylethyl ester (CA INDEX NAME)

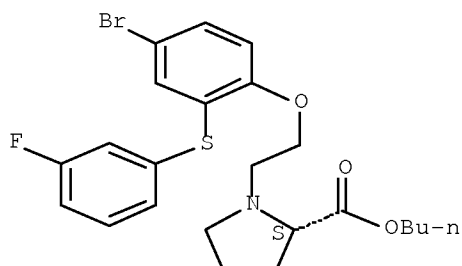
Absolute stereochemistry.



RN 791644-07-0 HCAPLUS

CN L-Proline, 1-[2-[4-bromo-2-[(3-fluorophenyl)thio]phenoxy]ethyl]-, butyl
ester (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/551737

***** QUERY RESULTS *****

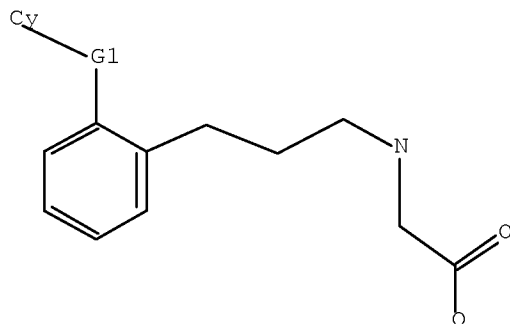
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(FILE 'HCAPLUS' ENTERED AT 13:11:11 ON 26 MAR 2009)

L24 9 S L15 NOT L23

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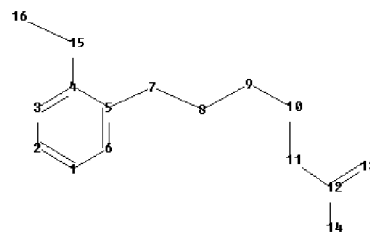
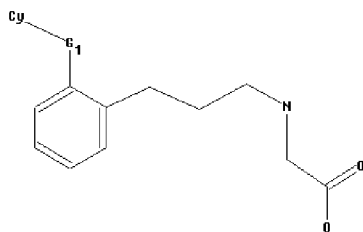
L5 STR



G1 O, S

Structure attributes must be viewed using STN Express query preparation:

Uploading L3.str



chain nodes :

7 12 13 14 15 16

ring nodes :

1 2 3 4 5 6

ring/chain nodes :

8 9 10 11

chain bonds :

4-15 5-7 7-8 11-12 12-13 12-14 15-16

ring/chain bonds :

8-9 9-10 10-11

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

4-15 8-9 9-10 10-11 12-13 12-14 15-16

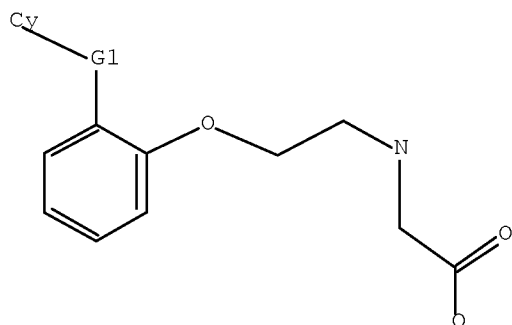
10/551737

exact bonds :
5-7 7-8 11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom
Generic attributes :
16:
Type of Ring System : Monocyclic

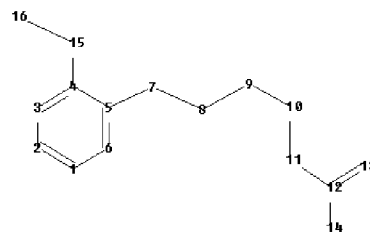
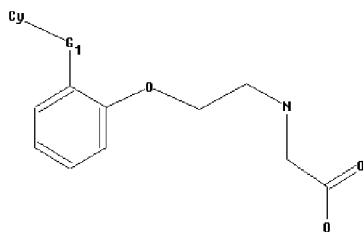
L9 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation:

Uploading L5.str



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chain nodes :
7 12 13 14 15 16
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
8 9 10 11
chain bonds :
4-15 5-7 7-8 11-12 12-13 12-14 15-16
ring/chain bonds :
8-9 9-10 10-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
4-15 5-7 7-8 8-9 9-10 10-11 12-13 12-14 15-16
exact bonds :
11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

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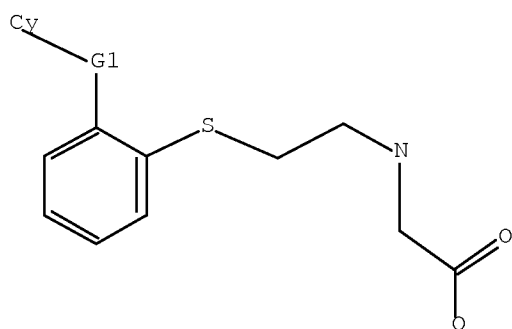
G1:O,S

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Match level :
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11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom
Generic attributes :
16:
Type of Ring System : Monocyclic

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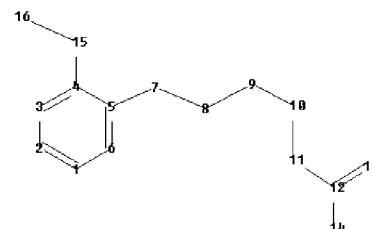
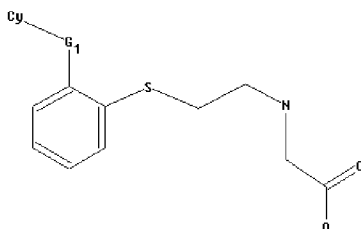
L11 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation:

Uploading L6.str



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chain nodes :
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ring nodes :
1 2 3 4 5 6
ring/chain nodes :
8 9 10 11
chain bonds :
4-15 5-7 7-8 11-12 12-13 12-14 15-16
ring/chain bonds :
8-9 9-10 10-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
4-15 5-7 7-8 8-9 9-10 10-11 12-13 12-14 15-16
exact bonds :
11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

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G1:O,S

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom

Generic attributes :

16:

Type of Ring System : Monocyclic

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L20      71 SEA FILE=HCAPLUS ABB=ON PLU=ON ANDERSEN KIM/AU
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L22      19 SEA FILE=HCAPLUS ABB=ON PLU=ON ESKILDSSEN J?/AU

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OR L22)) AND L15) OR (L15 AND L16)
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=> d l24 1-9 ibib abs hitstr

L24 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:1093266 HCAPLUS Full-text
DOCUMENT NUMBER: 145:432223
TITLE: Method of treating schizophrenia prodrome
INVENTOR(S): Woods, Scott W.
PATENT ASSIGNEE(S): Yale University, USA
SOURCE: PCT Int. Appl., 64pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006110724	A2	20061019	WO 2006-US13444	20060411
WO 2006110724	A3	20070322		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
AU 2006235400	A1	20061019	AU 2006-235400	20060411
CA 2602626	A1	20061019	CA 2006-2602626	20060411
EP 1871165	A2	20080102	EP 2006-740849	20060411
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU			
JP 2008535864	T	20080904	JP 2008-505637	20060411
PRIORITY APPLN. INFO.:			US 2005-670600P	P 20050411
			WO 2006-US13444	W 20060411

OTHER SOURCE(S): MARPAT 145:432223

AB The present invention relates to a method of treating schizophrenia prodrome in human subjects using a NMDA glycine site agonist, a glycine transporter-1 inhibitor or mixts. thereof, optionally in combination with a pharmaceutically acceptable additive, carrier or excipient.

IT 791642-83-6

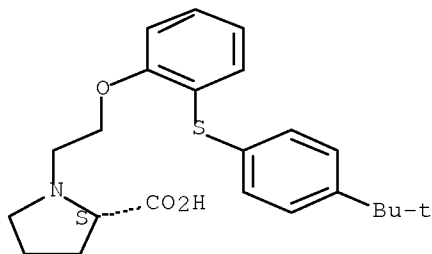
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(method of treating schizophrenia prodrome with NMDA glycine agonist and glycine transporter-1 inhibitor)

RN 791642-83-6 HCAPLUS

CN L-Proline, 1-[2-[2-[[4-(1,1-dimethylethyl)phenyl]thio]phenoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:1154515 HCAPLUS Full-text

DOCUMENT NUMBER: 143:422634

TITLE: Preparation of N-(2-aryloxyethyl)glycine derivatives and their use as glycine transport inhibitors

INVENTOR(S): Man, Teresa; Milot, Guy; Porter, Warren Jaye; Reel, Jon Kevin; Rudyk, Helene Catherine Eugenie; Valli, Matthew John; Walter, Magnus Wilhelm

PATENT ASSIGNEE(S): Eli Lilly and Company, USA

SOURCE: PCT Int. Appl., 187 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

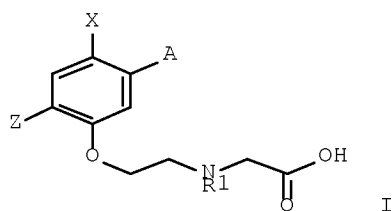
PATENT INFORMATION:

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WO 2005100301	A1	20051027	WO 2005-US8962	20050318
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

PRIORITY APPLN. INFO.: US 2004-558260P P 20040331

OTHER SOURCE(S): CASREACT 143:422634; MARPAT 143:422634

GI



AB The invention relates to (aryloxyethyl)glycine derivs. I [X is H, halo, alkyl, CF₃, cycloalkyl, arylcarbonyl, (un)substituted aryl, fused arylcycloalkyl or heteroaryl, fused arylheterocyclyl; Z is alkyl, alkenyl, Y, CO-Y, CH(OH)-Y, OY, alkyl-Y, alkyl-OY, SY, CF₂Y or NR₂-Y, where Y is alkyl, (CH₂)₁₋₁₀CF₃, CF₃, C₂F₅, C₃F₇, (un)substituted aryl, heteroaryl, cycloalkyl or heterocyclyl and R₂ is H or alkyl; A is (un)substituted aryl, H, alkoxy; R₁ is alkyl] or their pharmaceutically-acceptable salts that exhibit activity as inhibitors of the glycine type-1 transporter, to pharmaceutical compns. containing them and to their use in the treatment of neurol. and neuropsychiatric disorders. Thus, glycine derivative I (X = Ph, Z = 2-thienyl, A = H, R₁ = H) was prepared via reactions of 3-iodo-4-methoxybiphenyl, 2-thiopheneboronic acid, and [(2-hydroxyethyl)methylamino]acetic acid tert-Bu ester.

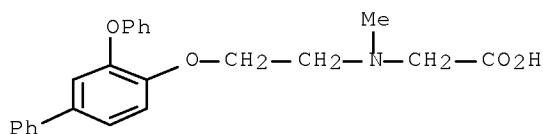
IT 868263-52-9P 868264-97-5P 868265-44-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of (aryloxyethyl)glycine derivs. as glycine transport inhibitors)

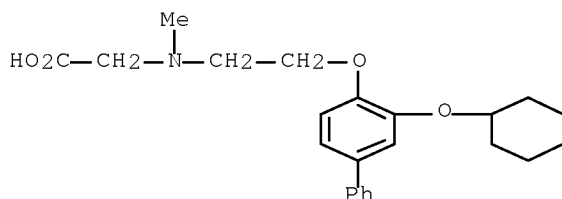
RN 868263-52-9 HCAPLUS

CN Glycine, N-methyl-N-[2-[(3-phenoxy[1,1'-biphenyl]-4-yl)oxy]ethyl]- (CA INDEX NAME)

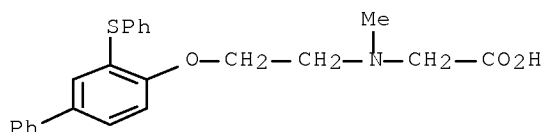


RN 868264-97-5 HCAPLUS

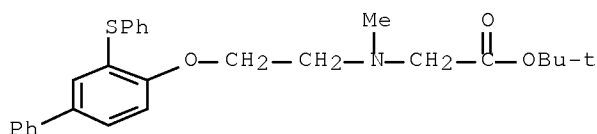
CN Glycine, N-[2-[[3-(cyclohexyloxy)[1,1'-biphenyl]-4-yl]oxy]ethyl]-N-methyl- (CA INDEX NAME)



RN 868265-44-5 HCAPLUS
 CN Glycine, N-methyl-N-[2-[[3-(phenylthio)[1,1'-biphenyl]-4-yl]oxy]ethyl]-
 (CA INDEX NAME)



IT 868263-20-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of (aryloxyethyl)glycine derivs. as glycine transport
 inhibitors)
 RN 868263-20-1 HCAPLUS
 CN Glycine, N-methyl-N-[2-[[3-(phenylthio)[1,1'-biphenyl]-4-yl]oxy]ethyl]-,
 1,1-dimethylethyl ester (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2004:878155 HCAPLUS Full-text
 DOCUMENT NUMBER: 141:366240
 TITLE: Preparation of pyrrolopyridazines for the treatment of
 proliferative disorders
 INVENTOR(S): Salvati, Mark E.; Illig, Carl R.; Wilson, Kenneth
 Jerome; Chen, Jinsheng; Meegalla, Sanath K.; Wall,
 Mark James
 PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
 SOURCE: U.S. Pat. Appl. Publ., 189 pp., Cont.-in-part of U.S.
 Ser. No. 396,197.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

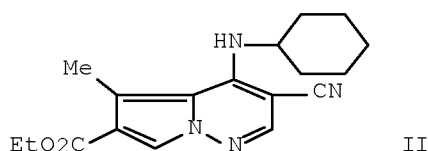
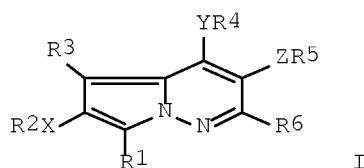
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20040209886	A1	20041021	US 2003-672850	20030926
US 7030112	B2	20060418		
US 20040063712	A1	20040401	US 2003-396197	20030325

US 6900208 B2 20050531
 WO 2005030144 A2 20050407 WO 2004-US31571 20040923
 WO 2005030144 A3 20051027

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
 CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
 GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
 LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
 NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
 TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
 AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
 EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
 SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
 SN, TD, TG

EP 1664051 A2 20060607 EP 2004-789070 20040923
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR
 US 20050159420 A1 20050721 US 2005-29547 20050105
 PRIORITY APPLN. INFO.: US 2003-396197 A2 20030325
 US 2002-368249P P 20020328
 US 2002-402118P P 20020808
 US 2003-672850 A 20030926
 WO 2004-US31571 W 20040923

OTHER SOURCE(S): MARPAT 141:366240
 GI



AB Pyrrolopyridazines I [R1 = H, alkyl, aralkyl, halo, OH, etc.; R2 = alkyl, cycloalkyl, aryl, heterocyclic, aralkyl, (un)substituted CO2H, CHO, CONH2, SO3H, SO2NH2, SH, S(O)H, SO2H; R1R2, R2R3 = cycloalkyl, aryl, heterocyclic; R3 = H, alkyl, cycloalkyl, heterocyclic, aryl, aralkyl, acyl, halo, (un)substituted OH, CH2OH, CH2NH2, CH2SH; R4 = alkyl, cycloalkyl, aryl, heterocyclic, aralkyl, acyl, (un)substituted CO2H, CONH2, SO3H, SO2NH2, SH, S(O)H, SO2H; R5 = H, halo, CN, alkyl, cycloalkyl, heterocyclic, aryl, aralkyl, acyl, alkylene, (un)substituted CO2H, CONH2, SO3H, SO2NH2, SH, S(O)H, SO2H; R6 = H, alkyl, cycloalkyl, aryl, aralkyl, heterocyclic, acyl, alkoxy carbonyl, carbamoyl; X, Y, Z = bond, O, S, (un)substituted NH, etc.] were prepared for use in the treatment of proliferative, inflammatory, and other disorders (no data). Thus, NCCCH2CO2Et was cyclized with MeCHO to di-Et 3-methyl-1H-pyrrole-2,4-dicarboxylate which was N-aminated and cyclized with (EtO)2CHCH2CN to give Et 3-cyano-1,4-dihydro-5-methyl-4-oxopyrrolo[1,2-b]pyridazine-6-carboxylate.

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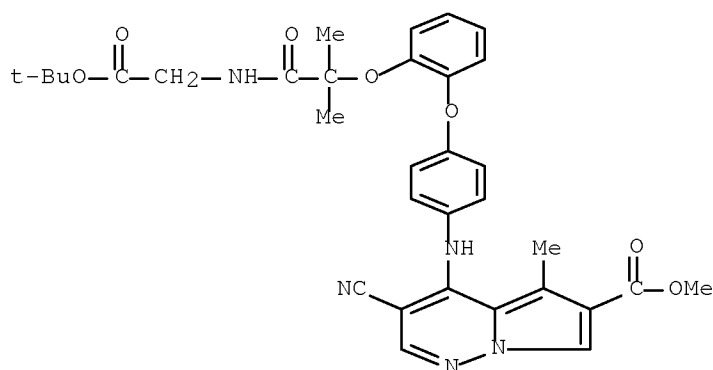
This ketone was chlorinated and treated with cyclohexylamine to give the title compound II. The compds. I were tested against several different kinases such as VEGFR-2, FGFR-1, HER-1, HER-2, HER-4, MEK and p38 kinases. Thus, tested compds. I inhibited VEGFR-2 and FGFR-1 kinases with IC50 of $\leq 80 \mu\text{M}$.

IT 779344-57-9P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of pyrrolopyridazines for the treatment of proliferative disorders)

RN 779344-57-9 HCAPLUS

CN Pyrrolo[1,2-b]pyridazine-6-carboxylic acid,
3-cyano-4-[[4-[2-[2-[[2-(1,1-dimethylethoxy)-2-oxoethyl]amino]-1,1-dimethyl-2-oxoethoxy]phenoxy]phenyl]amino]-5-methyl-, methyl ester (CA INDEX NAME)

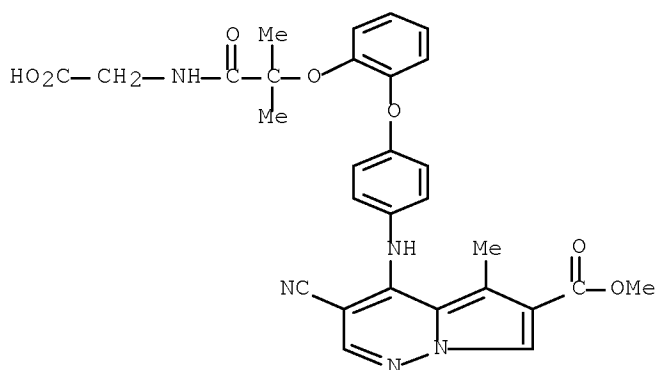


IT 779344-58-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrrolopyridazines for the treatment of proliferative disorders)

RN 779344-58-0 HCAPLUS

CN Pyrrolo[1,2-b]pyridazine-6-carboxylic acid,
4-[[4-[2-[2-[(carboxymethyl)amino]-1,1-dimethyl-2-oxoethoxy]phenoxy]phenyl]amino]-3-cyano-5-methyl-, 6-methyl ester (CA INDEX NAME)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:946033 HCAPLUS Full-text

DOCUMENT NUMBER: 138:20910

TITLE: Preparation of
3-Methyl-2,6-dioxo-4-(trifluoromethyl)-1,2,3,6-
tetrahydropyrimidine derivatives as plant growth
regulators for cotton

INVENTOR(S): Mito, Nobuaki

PATENT ASSIGNEE(S): Sumitomo Chemical Company, Limited, Japan

SOURCE: PCT Int. Appl., 78 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

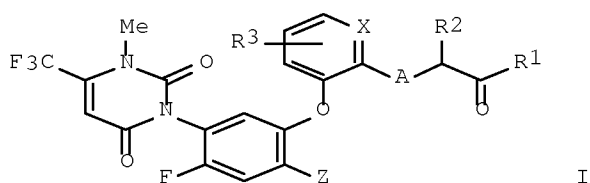
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002098227	A1	20021212	WO 2001-JP4584	20010531
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2001262676	A1	20021216	AU 2001-262676	20010531
AU 2001262676	B2	20070125		
BR 2001017032	A	20040420	BR 2001-17032	20010531
US 20040152597	A1	20040805	US 2003-476511	20031103
US 7115544	B2	20061003		

PRIORITY APPLN. INFO.: WO 2001-JP4584 W 20010531

OTHER SOURCE(S): MARPAT 138:20910

GI



AB Plant growth regulators for cotton containing as an active ingredient a compound I (X = CH, or N; Z = halo; A = O, S, or NH; R1 = OH, C1-C7 alkoxy, C3-C7 alkenyloxy, C3-C7 alkynyloxy, C5-C7 cycloalkoxy, [di(C1-C7 alkoxy)carbonyl]C1-C3 alkoxy, (C1-C7 alkylamino)oxy, [di(C1-C7 alkyl)amino]oxy, (C3-C7 alkylideneamino)oxy, C1-C7 alkylamino, di(C1-C7 alkyl)amino, C3-C7 alkenylamino, C3-C7 alkynylamino, C5-C7 cycloalkylamino, [(C1-C7 alkoxy)carbonyl]C1-C3 alkylamino, or (C1-C7 alkoxy)amino; R2 = H, or Me; R3 = H, halo, C1-C3 alkyl, or C1-C3 alkoxy) are prepared

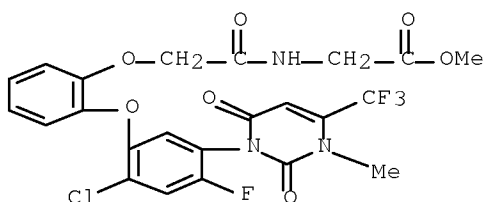
IT 380500-89-0P 477714-69-5P 477715-66-5P
477715-68-7P

RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation as plant growth regulator for cotton)

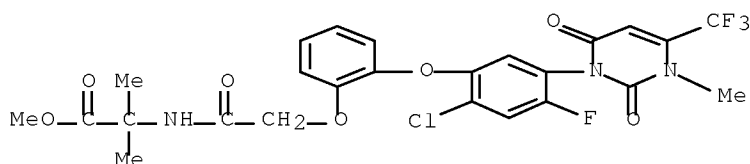
RN 380500-89-0 HCAPLUS

CN Glycine, N-[[2-[2-chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluorophenoxy]phenoxy]acetyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 477714-69-5 HCAPLUS

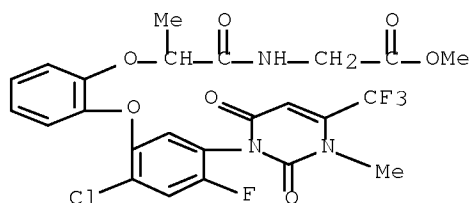
CN Alanine, N-[[2-[2-chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluorophenoxy]phenoxy]acetyl]-2-methyl-, methyl ester (9CI) (CA INDEX NAME)



RN 477715-66-5 HCAPLUS

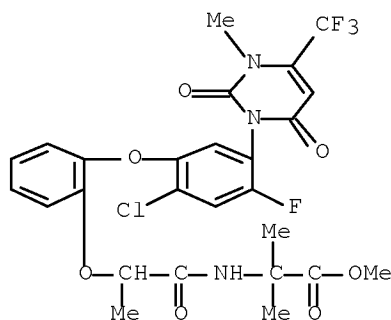
10/551737

CN Glycine, N-[2-[2-[2-chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluorophenoxy]phenoxy]-1-oxopropyl]-, methyl ester (CA INDEX NAME)



RN 477715-68-7 HCAPLUS

CN Alanine, N-[2-[2-[2-chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluorophenoxy]phenoxy]-1-oxopropyl]-2-methyl-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:428894 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 137:20303

TITLE: Preparation of substituted quinolines as antitumor agents

INVENTOR(S): Boyle, Francis Thomas; Gibson, Keith Hopkinson; Foote, Kevin Michael

PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca UK Limited

SOURCE: PCT Int. Appl., 118 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002044166	A1	20020606	WO 2001-GB4737	20011026
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				

10/551737

CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
 PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA,
 UG, US, UZ, VN, YU, ZA, ZW
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
 BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
 AU 2002010714 A 20020611 AU 2002-10714 20011026
 EP 1337524 A1 20030827 EP 2001-978616 20011026
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
 JP 2004514718 T 20040520 JP 2002-546536 20011026
 US 20040029898 A1 20040212 US 2003-415812 20030502
 US 7067532 B2 20060627
 US 20070021407 A1 20070125 US 2006-374423 20060314
 US 7402583 B2 20080722
 PRIORITY APPLN. INFO.: GB 2000-26744 A 20001102
 GB 2000-26746 A 20001102
 GB 2000-26747 A 20001102
 WO 2001-GB4737 W 20011026
 US 2003-415812 A3 20030502
 OTHER SOURCE(S): MARPAT 137:20303
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [n = 0 or 1; Y = NH, O, S, or alkylamine; R5 = CN, F, Cl, or Br; R6 = (un)substituted -cycloalkyl, -pyridinyl, -pyrimidinyl, -Ph, etc.; R1, R2 and R4 independently = H, OH, halo, CN, NO2, F3C, alkyl, amine, alkylamine, dialkylamine, R7X1(CH2)x- wherein x = 0-3, R7 = H, (un)substituted hydrocarbyl or heterocyclyl and X1 = O, CH2, OCO, CO, S, SO, SO2, NR8CO, NR8CO2, CONR9, CO2NR9, SO2NR10, NR11 or NR11NR11 wherein R8, R9, R10 and R11 independently = H, alkyl or alkoxyalkyl; R3 = group of formula X1R12(OH)p where p = 1-2 and R12 = alkylene, alkenylene or alkynylene chain, optionally interposed with a heteroatom or heterocyclic ring with the provision that when R12 = alkylene, R12 must be interposed with a heteroatom or heterocyclic ring and at least one (OH)p is on the alkylene chain between X1 and the interposed heteroatom or heterocyclic ring; group of formula R7(CH2)yX1(CH2)x where y = 0-5 and (CH2)y is optionally interposed by an X1 group; group of formula X1alkyl where alkyl is substituted by one or more Cl and/or CN; heterocyclic ring, etc.], or a pharmaceutically acceptable salt, pro-drug or solvate thereof are prepared and disclosed as antiproliferative agents. Thus, II was prepared in eight steps from benzylchloroformate and 2-methoxy-5-nitroaniline. I were evaluated as inhibitors of MAPK pathway and exhibited IC50 values typically less than 0.5 μ M, e.g., II possessed an IC50 = 0.0013 μ M. In cell proliferation assays, I had IC50 results typically less than 30 μ M with II giving an IC50 of 1.3 μ M in HT29 human colon tumor cells. Methods for prevention of cancer comprising administering an effective amount of compound I are further claimed.

IT 306999-95-1P 307309-82-6P

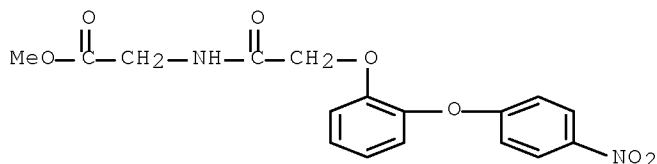
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation, inhibition of MAP kinase, and cellular antiproliferation activity of substituted quinolines as antitumor agents)

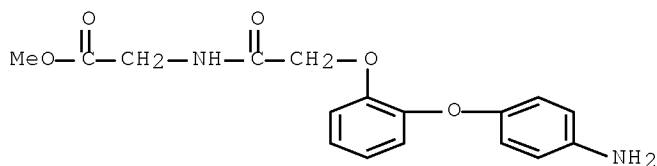
RN 306999-95-1 HCAPLUS

CN Glycine, N-[[2-(4-nitrophenoxy)phenoxy]acetyl]-, methyl ester (9CI) (CA

INDEX NAME)



RN 307309-82-6 HCAPLUS

CN Glycine, N-[[2-(4-aminophenoxy)phenoxy]acetyl]-, methyl ester (9CI) (CA
INDEX NAME)REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:353433 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 136:369616

TITLE: Preparation of 3-cyano-4-arylaminquinolines as
inhibitors of MAP kinase for use as antitumor agents

INVENTOR(S): Boyle, Francis Thomas; Gibson, Keith Hopkinson

PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca UK Limited

SOURCE: PCT Int. Appl., 149 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2002036570	A1	20020510	WO 2001-GB4733	20011025
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2001095791	A	20020515	AU 2001-95791	20011025
EP 1337513	A1	20030827	EP 2001-976523	20011025

10/551737

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

JP 2004517059	T	20040610	JP 2002-539330	20011025
US 20050101630	A1	20050512	US 2003-415813	20030502
US 7253184	B2	20070807		
US 20080027054	A1	20080131	US 2007-826507	20070716
US 7504416	B2	20090317		

PRIORITY APPLN. INFO.: GB 2000-26745 A 20001102
 GB 2000-26747 A 20001102
 WO 2001-GB4733 W 20011025
 US 2003-415813 A3 20030502

OTHER SOURCE(S): MARPAT 136:369616
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. I [R1, R2, R3, R4 independently H, HO, halogen, NC, O2N, F3C, (un)substituted C1-C3 alkyl, (un)substituted amino, saturated heterocyclyl containing two heteroatoms; R5 = NC, F, Cl, Br; R6 = divalent C1-C5 alkenyl, C3-C7 cycloalkyl, or heteroaryl moiety; R7 = AR8; A = bond, O, CO, S, SO, SO2, (un)substituted aminocarbonyl, (un)substituted carbonylamino, (un)substituted sulfonylamino, (un)substituted aminosulfonyl, (un)substituted amino; R8 = C1-C6 alkyl, C2-C6 alkenyl, C2-C6 alkynyl; R9 = (un)substituted C3-C7 divalent cycloalkyl; R10 = (un)substituted arylene, heteroarylene, heteroarylene N-oxide, C3-C10 cycloalkylene; X = amino, (C1-C6)alkylamino, O, S, CH2; Y = amino, (C1-C6)alkylamino, O, S; Z = (un)substituted alkyl, alkylene, alkynylene, O, CO, COO, S, SO, SO2, (un)substituted aminocarbonyl, carbonylamino, sulfonylamino, aminosulfonyl, amino; n = 0,1; m and p independently 0-3; alternatively, R10Z(CH2)pR6R7 can be replaced with a heteroaryl or heterocyclyl-2,3-fused Ph ring] were prepared as inhibitors of MAP kinase for use as antitumor agents. E.g., 1-fluoro-4-nitrobenzene undergoes nucleophilic substitution with (2-hydroxyphenoxy)acetic acid followed by coupling of the acid with Me glycinate, reduction of the nitro group with Pd/C, and reaction of the ester with N-methylpiperazine to give the aminophenoxymethylcarbonylaminoacetyl piperazine II. E.g., coupling of II with 4-chloro-6,7-dimethoxy-3-quinolinenitrile gave the example compound III. Biol. data was obtained for selected compds. Selected compds. inhibited MAP kinase with IC50 < 0.5 µM; for example, III gave an IC50 of 3.8 nM. In addition, selected compds. inhibited the proliferation of human colon cancer cells with IC50 < 30 µM; for example, III gave an IC50 of 1 µM.

IT ~~423179-57-1P~~

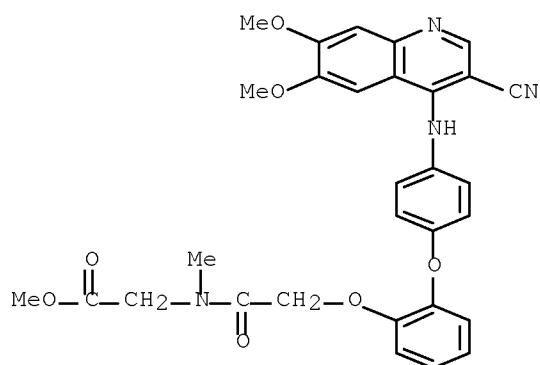
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(example compds.; preparation of 4-arylamino-3-cyanoquinolines as inhibitors

of MAP kinase for potential use as antitumor agents)

RN 423179-57-1 HCAPLUS

CN Glycine, N-[[2-[4-[(3-cyano-6,7-dimethoxy-4-quinolinyl)amino]phenoxy]phenoxy]acetyl]-N-methyl-, methyl ester (9CI)
 (CA INDEX NAME)



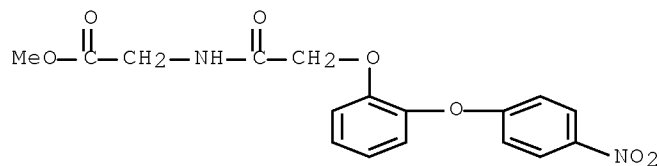
IT 306999-95-1P 307309-82-6P 423180-30-7P
 423180-31-8P 423180-57-8P 423180-59-0P
 423180-89-6P 423180-90-9P 423180-96-5P
 423180-97-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(intermediates; preparation of 4-aryl-amino-3-cyanoquinolines as inhibitors
 of MAP kinase for potential use as antitumor agents)

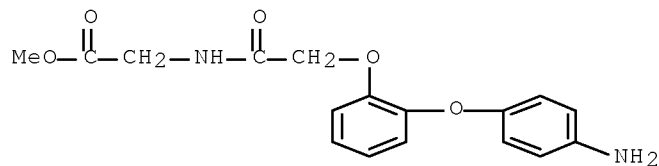
RN 306999-95-1 HCAPLUS

CN Glycine, N-[[2-(4-nitrophenoxy)phenoxy]acetyl]-, methyl ester (9CI) (CA
 INDEX NAME)



RN 307309-82-6 HCAPLUS

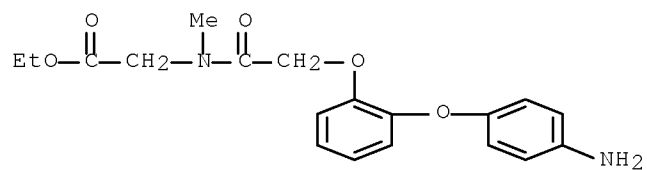
CN Glycine, N-[[2-(4-aminophenoxy)phenoxy]acetyl]-, methyl ester (9CI) (CA
 INDEX NAME)



RN 423180-30-7 HCAPLUS

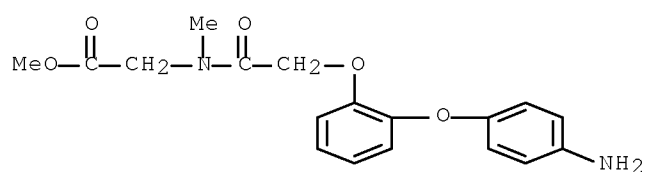
CN Glycine, N-[[2-(4-aminophenoxy)phenoxy]acetyl]-N-methyl-, ethyl ester
 (9CI) (CA INDEX NAME)

10/551737



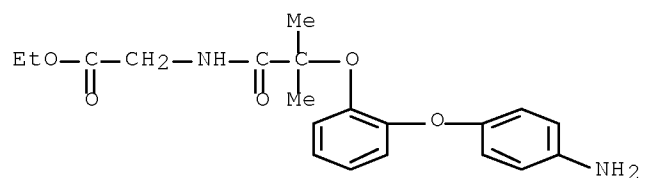
RN 423180-31-8 HCAPLUS

CN Glycine, N-[[2-(4-aminophenoxy)phenoxy]acetyl]-N-methyl-, methyl ester
(9CI) (CA INDEX NAME)



RN 423180-57-8 HCAPLUS

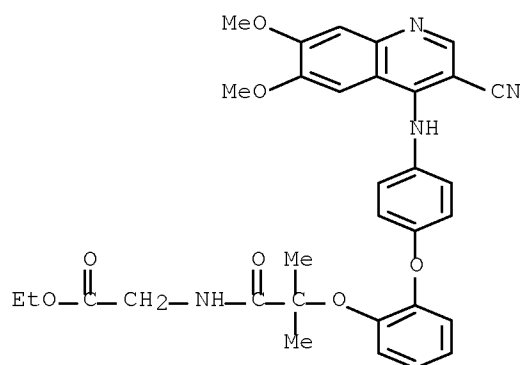
CN Glycine, N-[2-[2-(4-aminophenoxy)phenoxy]-2-methyl-1-oxopropyl]-, ethyl ester
(CA INDEX NAME)



RN 423180-59-0 HCAPLUS

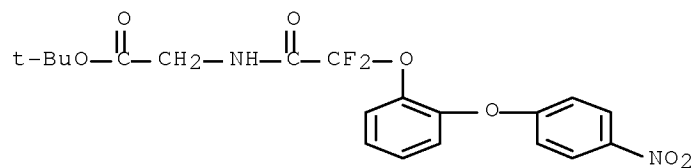
CN Glycine, N-[2-[2-[4-[(3-cyano-6,7-dimethoxy-4-quinolinyl)amino]phenoxy]phenoxy]-2-methyl-1-oxopropyl]-, ethyl ester
(CA INDEX NAME)

10/551737



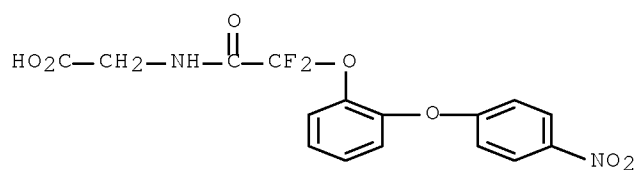
RN 423180-89-6 HCAPLUS

CN Glycine, N-[difluoro[2-(4-nitrophenoxy)phenoxy]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



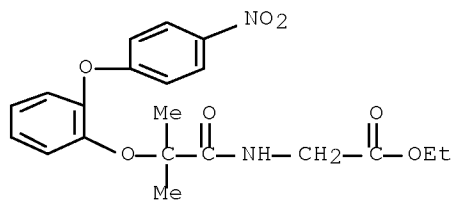
RN 423180-90-9 HCAPLUS

CN Glycine, N-[difluoro[2-(4-nitrophenoxy)phenoxy]acetyl]- (9CI) (CA INDEX NAME)

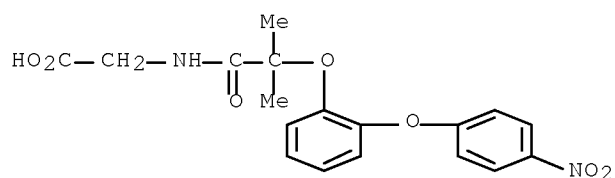


RN 423180-96-5 HCAPLUS

CN Glycine, N-[2-methyl-2-[2-(4-nitrophenoxy)phenoxy]-1-oxopropyl]-, ethyl ester (CA INDEX NAME)



RN 423180-97-6 HCAPLUS
 CN Glycine, N-[2-methyl-2-[2-(4-nitrophenoxy)phenoxy]-1-oxopropyl]- (CA INDEX NAME)

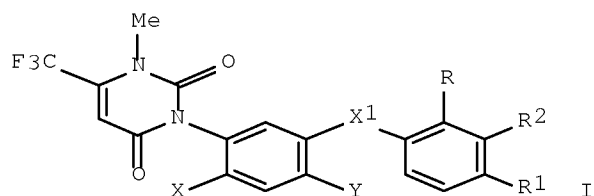


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2001:910259 HCAPLUS Full-text
 DOCUMENT NUMBER: 136:53754
 TITLE: Preparation and application of uracils as herbicides
 INVENTOR(S): Goto, Tomohiko; Sanemitsu, Minoru
 PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 91 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001348376	A	20011218	JP 2000-170234	20000607
PRIORITY APPLN. INFO.:			JP 2000-170234	20000607
OTHER SOURCE(S):	MARPAT 136:53754			

GI



AB Title compds. [I; R = OCH(CH₃)COOCH₂COOCH₃, (S)-OCH₂CONHCH(CH₂CH(CH₃)₂)CO₂CH₃, OCH₂CONHCH₂CO₂CH₃, OCH₂CO₂CH₂CO₂CH₃, OCH₂CO₂C(CH₃)₂CO₂CH₂CH:CH₂, H, CF₃, CH₃; R₁ = H, OCH(CH₃)CO₂CH₂COOH, OCH₂COOCH₂COOCH₂CH:CH₂, H; R₂ = H, OCH(CH₃)CO₂CH₂COOH, OCH₂COOCH₂COSCH₂CH₃; X = F, H; Y = Cl, NO₂; X₁ = O, S, NH] are prepared as herbicides. Thus, the title compound I (R = OCH₂COOC(CH₃)₂COOCH₂CH₂CH:CH₂; R₁ = H; R₂ = H; X = F; X₁ = O; Y = Cl) was prepared and field tested as effective herbicide in forage and soil treatment.

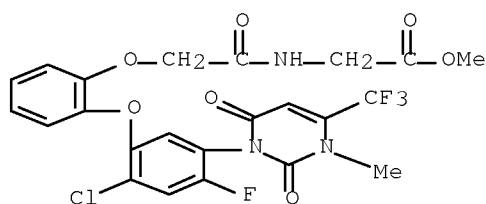
IT 380500-89-0P 380500-90-3P

RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and application of uracils as herbicides)

RN 380500-89-0 HCAPLUS

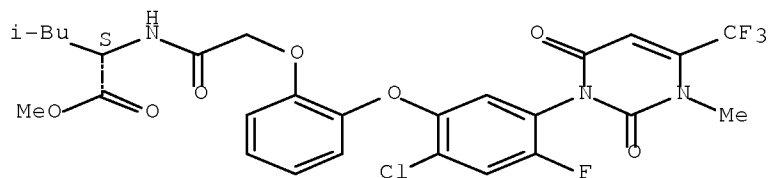
CN Glycine, N-[[[2-[2-chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluorophenoxy]phenoxy]acetyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 380500-90-3 HCAPLUS

CN L-Leucine, N-[[[2-[2-chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluorophenoxy]phenoxy]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:814464 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 133:362712

TITLE: Preparation of quinoline derivatives as inhibitors of MEK enzymes

INVENTOR(S): Boyle, Francis Thomas; Gibson, Keith Hopkinson; Poyser, Jeffrey Philip; Turner, Paul

PATENT ASSIGNEE(S): Astrazeneca AB, Swed.

SOURCE: PCT Int. Appl., 187 pp.

10/551737

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000068201	A1	20001116	WO 2000-GB1697	20000503
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2372663	A1	20001116	CA 2000-2372663	20000503
EP 1178967	A1	20020213	EP 2000-927491	20000503
EP 1178967	B1	20060308		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY				
TR 200103186	T2	20020422	TR 2001-3186	20000503
BR 2000010391	A	20020702	BR 2000-10391	20000503
HU 2002001219	A2	20020928	HU 2002-1219	20000503
HU 2002001219	A3	20030528		
EE 200100589	A	20030217	EE 2001-589	20000503
NZ 514980	A	20031031	NZ 2000-514980	20000503
AU 772846	B2	20040506	AU 2000-45891	20000503
CN 1219768	C	20050921	CN 2000-809959	20000503
EP 1584619	A1	20051012	EP 2005-13587	20000503
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, LV, FI, MK, CY, AL				
AT 319688	T	20060315	AT 2000-927491	20000503
PT 1178967	T	20060630	PT 2000-927491	20000503
ES 2258455	T3	20060901	ES 2000-927491	20000503
ZA 2001008971	A	20030130	ZA 2001-8971	20011030
IN 2001MN01338	A	20050304	IN 2001-MN1338	20011031
BG 106073	A	20020531	BG 2001-106073	20011101
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MX 2001011360	A	20020311	MX 2001-11360	20011107
PRIORITY APPLN. INFO.:			GB 1999-10577	A 19990508
			EP 2000-927491	A3 20000503
			WO 2000-GB1697	W 20000503
OTHER SOURCE(S):			MARPAT 133:362712	
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. [I; or a pharmaceutically acceptable salt thereof wherein: n is 0-1; X and Y are independently selected from NH, O, S, or NR8 where R8 is alkyl of 1-6 carbon atoms and X may addnl. comprise a CH2 group; R7 is a group (CH2)mR9 where m is 0, or an integer of from 1-3 and R9 is a substituted aryl group, an optionally substituted cycloalkyl ring of up to 10 carbon atoms, or an optionally substituted heterocyclic ring or an N-oxide of any nitrogen containing ring; R6 is a divalent cycloalkyl of 3 to 7 carbon atoms, which may

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be optionally further substituted with one or more alkyl of 1 to 6 carbon atom groups; or is a divalent pyridinyl, pyrimidinyl, or Ph ring; wherein the pyridinyl, pyrimidinyl, or Ph ring may be optionally further substituted with one or more specified groups; R1, R2, R3 and R4 are each independently selected from hydrogen or various specified organic groups]. Title compds. are useful as pharmaceuticals for the inhibition of MEK activity. Thus, the title compound II was prepared and tested in HT29 human colon tumor cell proliferation assay.

IT 306999-63-3P 306999-65-5P

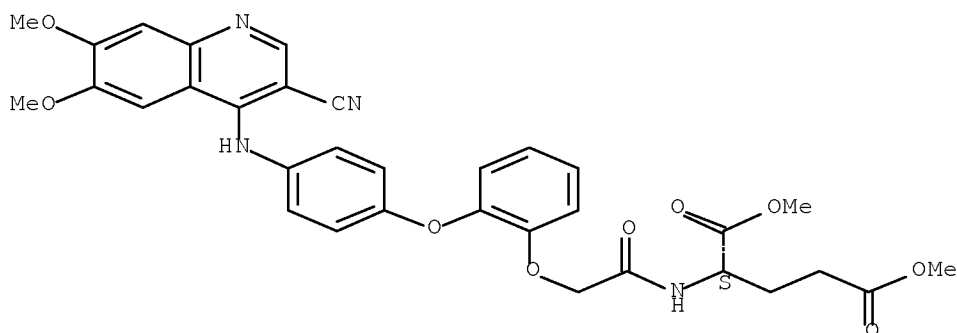
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of quinoline derivs. as inhibitors of MEK enzymes)

RN 306999-63-3 HCAPLUS

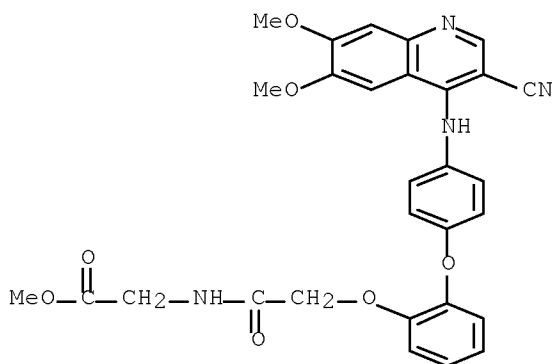
CN L-Glutamic acid, N-[[2-[4-[(3-cyano-6,7-dimethoxy-4-quinolinyl)amino]phenoxy]phenoxy]acetyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 306999-65-5 HCAPLUS

CN Glycine, N-[[2-[4-[(3-cyano-6,7-dimethoxy-4-quinolinyl)amino]phenoxy]phenoxy]acetyl]-, methyl ester (9CI) (CA INDEX NAME)



IT 306999-81-5 306999-85-9

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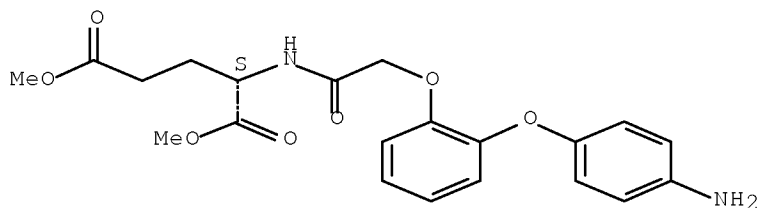
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of quinoline derivs. as inhibitors of MEK enzymes)

RN 306999-81-5 HCAPLUS

CN L-Glutamic acid, N-[[2-(4-aminophenoxy)phenoxy]acetyl]-, dimethyl ester
(9CI) (CA INDEX NAME)

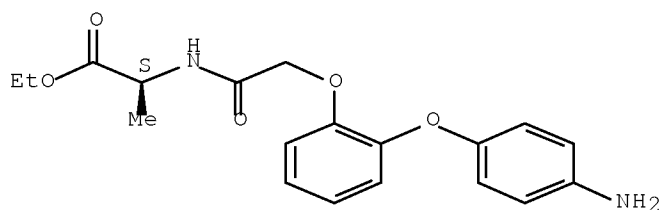
Absolute stereochemistry.



RN 306999-85-9 HCAPLUS

CN L-Alanine, N-[[2-(4-aminophenoxy)phenoxy]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 306999-93-9P 306999-95-1P 306999-96-2P
307309-82-6P

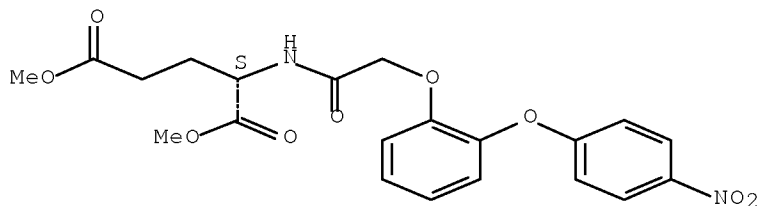
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(preparation of quinoline derivs. as inhibitors of MEK enzymes)

RN 306999-93-9 HCAPLUS

CN L-Glutamic acid, N-[[2-(4-nitrophenoxy)phenoxy]acetyl]-, dimethyl ester
(9CI) (CA INDEX NAME)

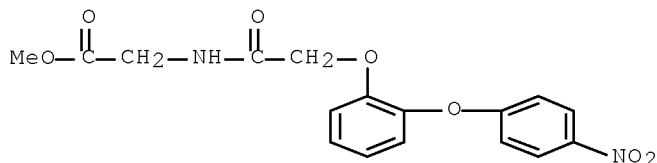
Absolute stereochemistry.



10/551737

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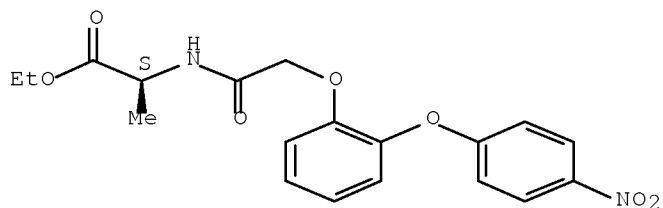
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RN 306999-96-2 HCAPLUS

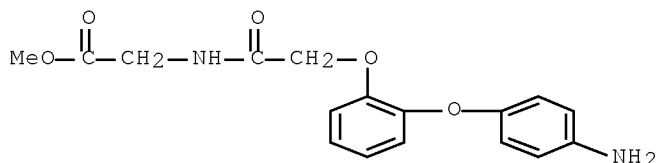
CN L-Alanine, N-[[2-(4-nitrophenoxy)phenoxy]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 307309-82-6 HCAPLUS

CN Glycine, N-[[2-(4-aminophenoxy)phenoxy]acetyl]-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1973:64458 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 78:64458

ORIGINAL REFERENCE NO.: 78:10181a,10184a

TITLE: Detection of alkali metal ions by optical rotatory dispersion. Sensitive test for sodium in the presence of lithium and potassium

AUTHOR(S): Wudl, Fred

CORPORATE SOURCE: Dep. Chem., State Univ. N. Y., Buffalo, NY, USA

SOURCE: Journal of the Chemical Society, Chemical Communications (1972), (22), 1229-30
CODEN: JCCCAT; ISSN: 0022-4936

DOCUMENT TYPE: Journal

LANGUAGE: English

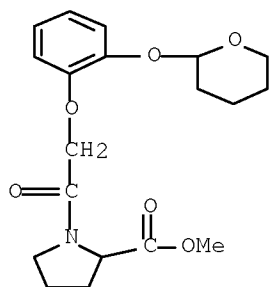
GI For diagram(s), see printed CA Issue.

AB The ORD curves of the chiral semicrown complexes (I, M = H, Li, Na, K) depend on the cation (M) and, as the interaction of I its strongest with Na, a spectropolarimetric determination of Na in the presence of Li and K is applicable.

IT 40418-12-0P
RL: PREP (Preparation)
(preparation of)

RN 40418-12-0 HCAPLUS

CN Proline, 1-[[2-[(tetrahydro-2H-pyran-2-yl)oxy]phenoxy]acetyl]-, methyl ester (9CI) (CA INDEX NAME)



10/551737

***** SEARCH HISTORY *****

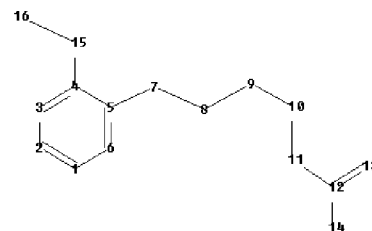
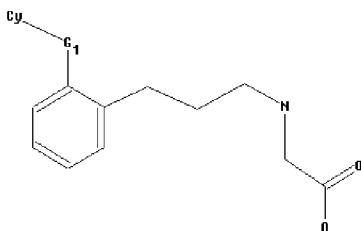
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FILE 'REGISTRY' ENTERED AT 12:47:46 ON 26 MAR 2009

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L3 STRUCTURE UPLOADED
 D
L4 0 SEA SSS SAM L3
L5 STRUCTURE UPLOADED
 D
L6 0 SEA SSS SAM L5
L7 STRUCTURE UPLOADED
 D

Uploading L3.str



chain nodes :
7 12 13 14 15 16
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
8 9 10 11
chain bonds :
4-15 5-7 7-8 11-12 12-13 12-14 15-16
ring/chain bonds :
8-9 9-10 10-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
4-15 8-9 9-10 10-11 12-13 12-14 15-16
exact bonds :
5-7 7-8 11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:O,S

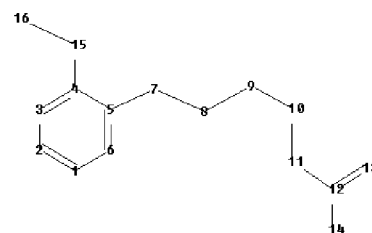
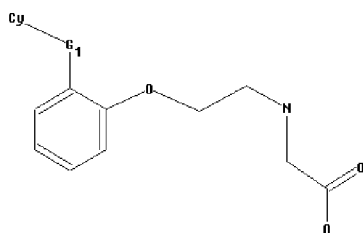
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10/551737

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom
Generic attributes :
16:
Type of Ring System : Monocyclic

L8 0 SEA SSS SAM L7
L9 STRUCTURE UPLOADED
D

Uploading L5.str



chain nodes :
7 12 13 14 15 16
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
8 9 10 11
chain bonds :
4-15 5-7 7-8 11-12 12-13 12-14 15-16
ring/chain bonds :
8-9 9-10 10-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
4-15 5-7 7-8 8-9 9-10 10-11 12-13 12-14 15-16
exact bonds :
11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:O,S

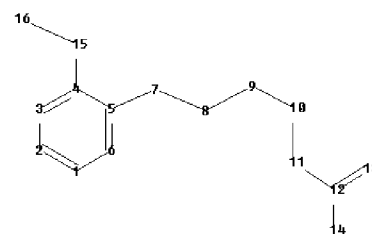
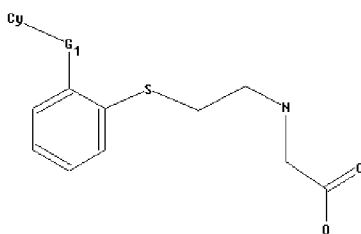
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom
Generic attributes :
16:

10/551737

Type of Ring System : Monocyclic

L10 1 SEA SSS SAM L9
L11 STRUCTURE UPLOADED

Uploading L6.str



chain nodes :
7 12 13 14 15 16
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
8 9 10 11
chain bonds :
4-15 5-7 7-8 11-12 12-13 12-14 15-16
ring/chain bonds :
8-9 9-10 10-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
4-15 5-7 7-8 8-9 9-10 10-11 12-13 12-14 15-16
exact bonds :
11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom
Generic attributes :
16:
Type of Ring System : Monocyclic

```

L12          0 SEA SSS SAM L11
L13          0 SEA SSS SAM L5 OR L9 OR L11
L14         171 SEA SSS FUL L5 OR L9 OR L11
              SAVE TEMP L14 BIA737REGCOM/A

FILE 'HCAPLUS' ENTERED AT 13:11:11 ON 26 MAR 2009
L15          11 SEA ABB=ON PLU=ON L14
L16          1 SEA ABB=ON PLU=ON US20060235003/PN
L17         11570 SEA ABB=ON PLU=ON SMITH G?/AU
L18          6 SEA ABB=ON PLU=ON SMITH GARRICK/AU
L19         17 SEA ABB=ON PLU=ON MIKKELSEN G?/AU
L20         71 SEA ABB=ON PLU=ON ANDERSEN KIM/AU
L21        203 SEA ABB=ON PLU=ON GREVE D?/AU
L22         19 SEA ABB=ON PLU=ON ESKILDSSEN J?/AU
L23          2 SEA ABB=ON PLU=ON (((L18 OR L19 OR L20 OR L21 OR L22)) AND
              L15) OR (L15 AND L16)
L24          9 SEA ABB=ON PLU=ON L15 NOT L23
              SAVE TEMP L23 BIA737HCAIN/A
              SAVE TEMP L24 BIA737HCAP/A
              D QUE L23
              D L23 1-2 IBIB ABS HITSTR
              D QUE L24
              D L24 1-9 IBIB ABS HITSTR

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